

WORKSHOP

“NSLS UPGRADES”

**Location:
BERKNER HALL
Room B**

You are invited to attend a workshop to discuss the near and long term development of the NSLS.

DATE: October 23, 2000

TIME: 8:30 am – 5:00 pm

HOST: Sam Krinsky

WORKSHOP ON NSLS UPGRADES
Berkner Hall, Room B
Monday, October 23, 2000

| | |
|--|-------|
| ◆ CONTINENTAL BREAKFAST..... | 8:00 |
| ◆ Introduction - Jack Marburger and Rick Osgood..... | 8:30 |
| ◆ What is the NSLS? | |
| Overview - S. Krinsky | 8:45 |
| NSLS compared to the world - S. Hulbert..... | 9:30 |
| Science with synchrotron radiation - C.C. Kao | 9:50 |
| BREAK..... | 10:20 |
| Improvements to existing facility - P. Siddons..... | 10:35 |
| DISCUSSION..... | 11:15 |
| ◆ Upgrade Options to be Discussed: | |
| Increase current in X-ray Ring using B-Factory technology | |
| B-Factory Upgrade, accelerator - E. Blum..... | 11:35 |
| B-Factory Upgrade, science - L. Berman..... | 11:55 |
| DISCUSSION..... | 12:15 |
| LUNCH (Berkner Hall, Room A)..... | 12:30 |
| Construction of a new storage ring of conventional design, such as | |
| Diamond or the Swiss Light Source | |
| New Storage Ring, accelerator- J.B. Murphy | 1:30 |
| New Storage Ring, science - E. Johnson | 1:50 |
| DISCUSSION..... | 2:10 |
| Construction of linac-based sources | |
| Energy-Recovery Linac Sources - I. Ben-Zvi..... | 2:30 |
| DISCUSSION..... | 3:00 |
| BREAK..... | 3:10 |
| Free-Electron Lasers - L.H. Yu | 3:25 |
| Science - J. Hastings | 3:55 |
| DISCUSSION..... | 4:35 |
| ◆ Summary and Wrap Up - Peter Paul..... | 4:50 |

What is the NSLS?

“Overview”

Samuel Krinsky

NSLS Upgrade Workshop

OVERVIEW

UPGRADE GOALS INTRODUCTION TO SYNCH. RAD. ACCELERATOR DEVELOPMENT

**S. Krinsky
October 23, 2000**

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GOALS: NSLS UPGRADE

- Keep NSLS vital and competitive for next five years
- Assure NSLS is a leading synchrotron radiation facility 5-10 years from now

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KEY ISSUES: NSLS UPGRADE

- Short term:
 1. Address reduction of PRT support for beamlines
 2. Upgrade old beamline optical components
 3. Upgrade storage ring hardware,
 4. Upgrade insertion devices

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KEY ISSUES: NSLS UPGRADE

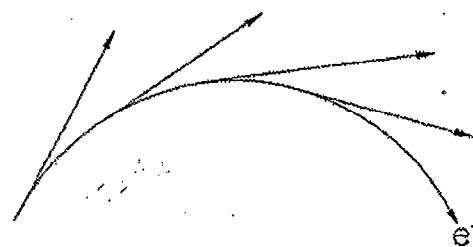
- Long term, provide:
 1. more straight sections for insertion devices;
 2. a source with smaller emittance, higher brightness;
 3. hard x-ray undulators;
 4. femtosecond x-rays;
 5. coherent (laser-like) sources.

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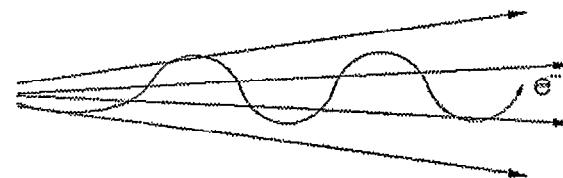
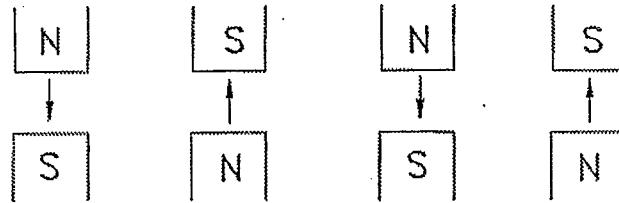
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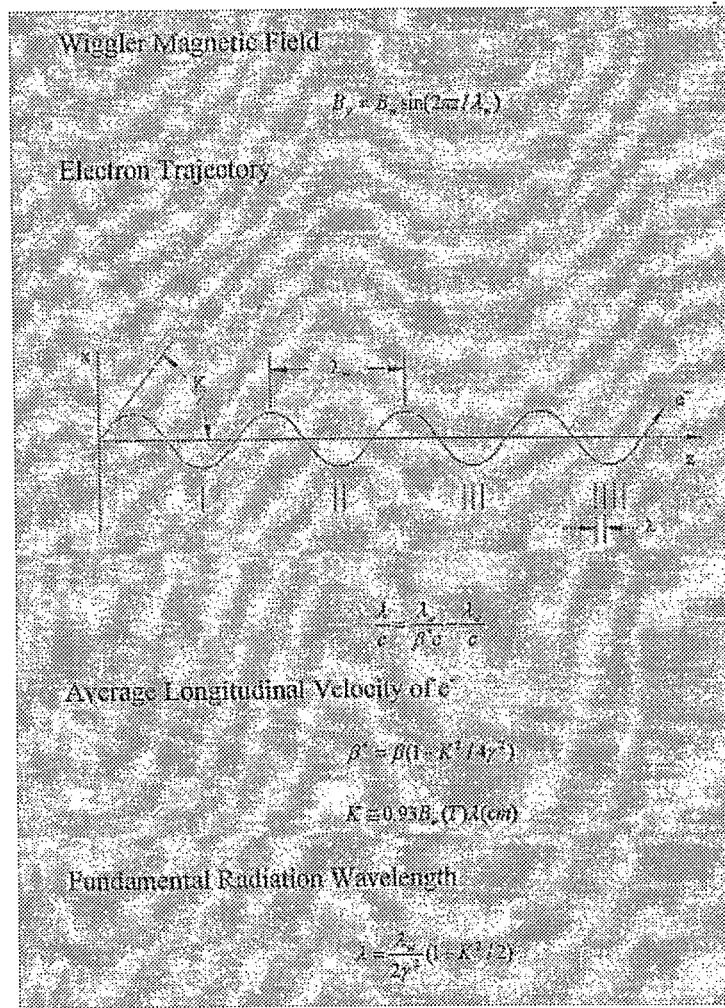
BENDING MAGNET

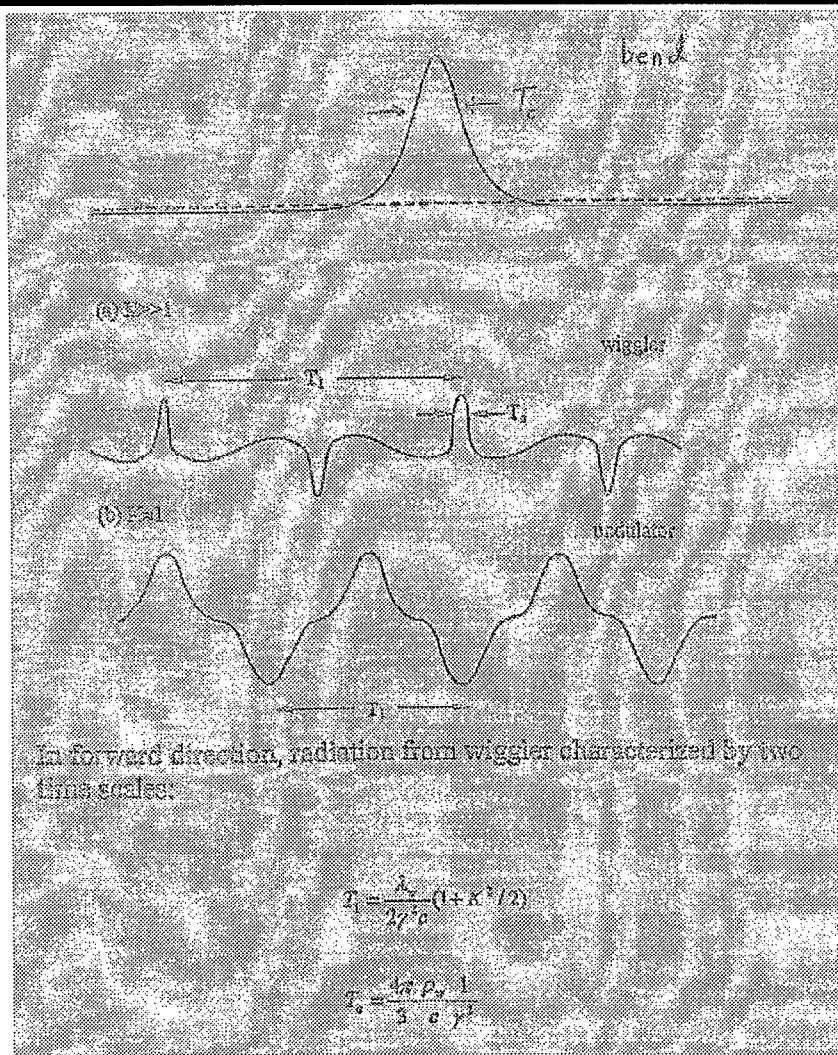


WIGGLER MAGNET

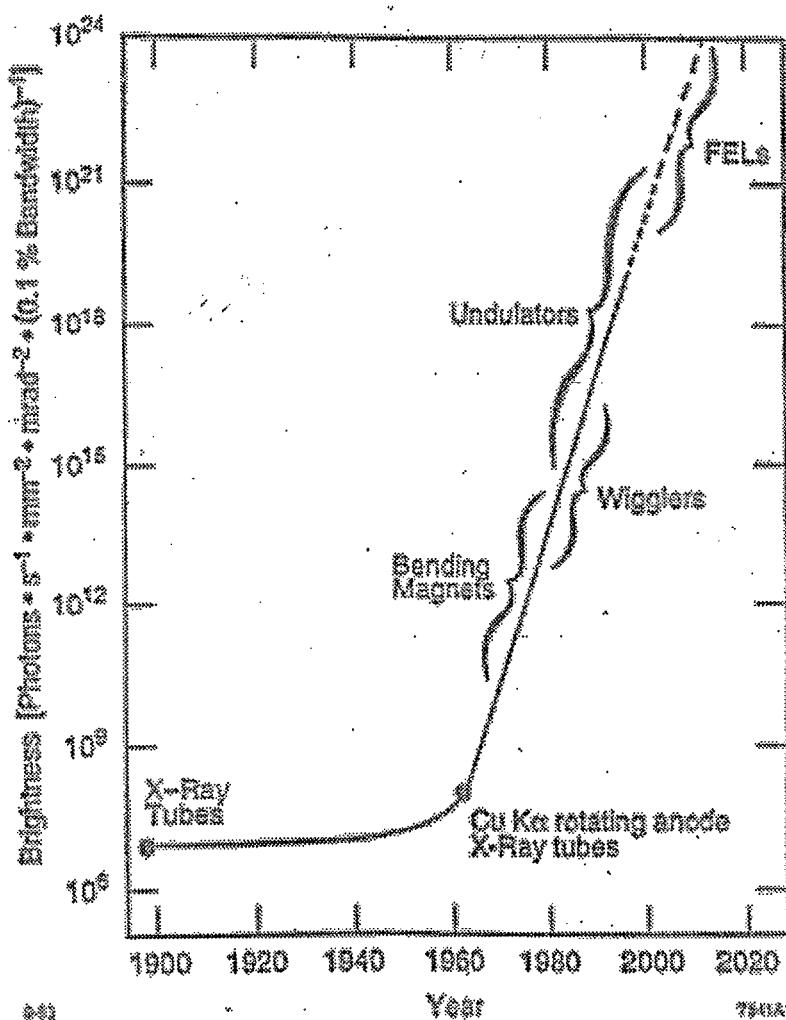


INCREASE PHOTONS PER UNIT SOLID ANGLE





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NSLS ACCELERATOR DEVELOPMENT

- Chasman-Green Lattice
- Brightness Optimization
- Bittner-Biscardi BPM Receivers
- Global Orbit Feedback Systems
- Infrared Sources
- Small Gap Undulators
- Time-Varying Elliptically Polarized Wiggler
- BNL Photocathode RF Gun
- High-Gain Harmonic-Generation Free-Electron Laser

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NSLS DESIGN PHILOSOPHY

G.K. Green: Maximize Source Brightness
Photons/Sec/Phase Space Volume/Bandwidth

Require high brightness to have parallel
photon beam incident on small sample

Design storage ring with small emittance

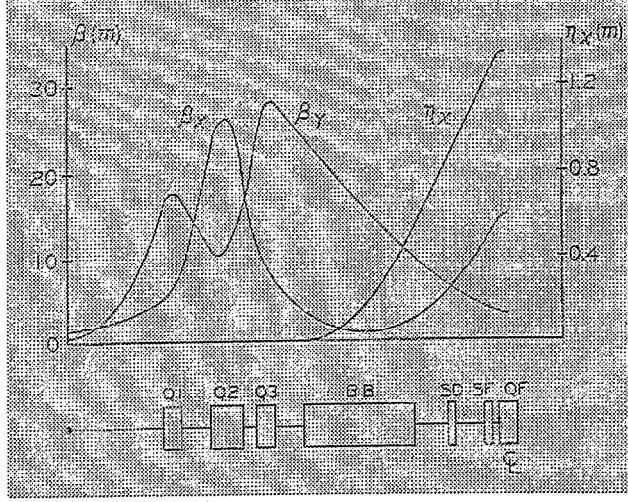
Chasman-Green Lattice:

Achromatic bends with zero dispersion
straights for insertion devices

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Undulator Brightness

$$\lambda = (c/2\pi) \times 10^{-12} \text{ cm}$$

$$B = \frac{2 \times 10^2}{v_e (\text{nm} \cdot \text{rad})} \cdot \frac{N_e K^2}{(1 + K^2/2)} \cdot \frac{N_e K^2}{(\text{ph}/0.1\%, \text{nm}, \text{nrad}^2, \text{Amp})}$$

$$v_e = (7.7 \times 10^{-10} \text{ nm} \cdot \text{rad}) \cdot \frac{1}{\lambda}$$

(Chasman-Green Lattice)

$$C = C_e / \gamma$$

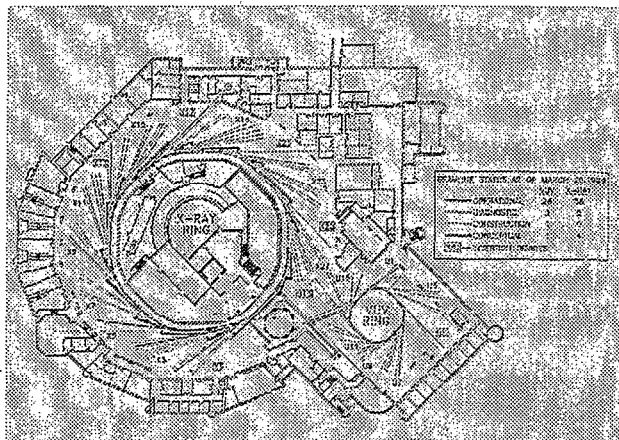
$$C_e = (1 - 4) \text{ nm} \cdot \text{nrad}$$

(max)

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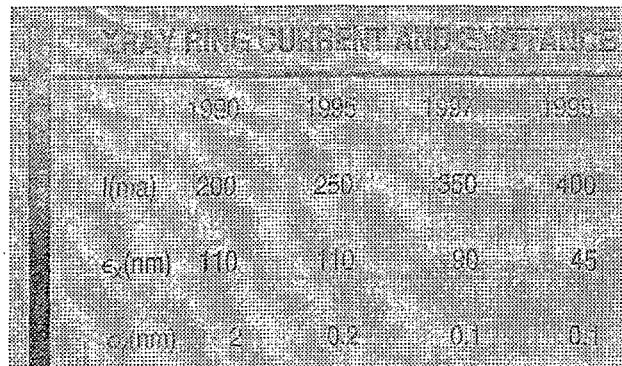
INSERTION DEVICES

- X1: Soft X-ray Undulator
 - Microscopy/Spectroscopy
- X5: LEGS – Nuclear Physics
- X13: R&D – Small Gap/Elliptically Polarized
- X17: Superconducting Wiggler – Medical,
High Pressure, Material Science
- X21: Hybrid Wiggler – Inelastic Scattering
- X25: Hybrid Wiggler – Protein
Crystallography/Scattering
- U5: Spin Polarized Photoemission
- U13: Soft X-ray Spectroscopy/5-30eV Source
- Infrared Bending Magnet Sources:
U2, U4IR, U10,U12
- X9, X29: New In-Vacuum Undulators

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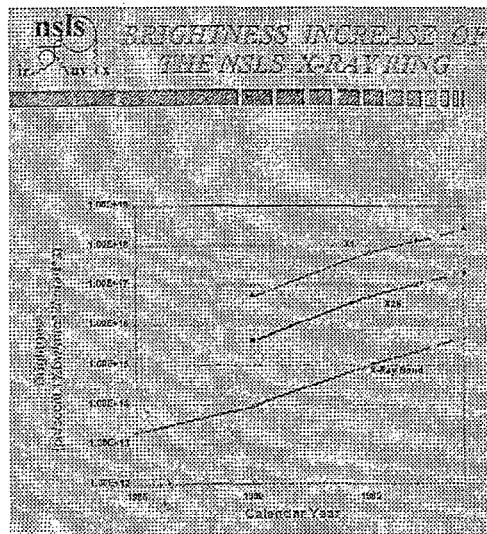
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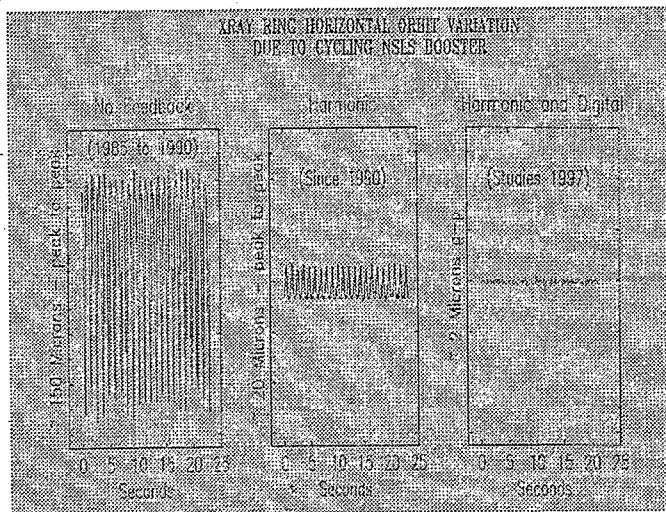


GLOBAL ORBIT FEEDBACK SYSTEMS

- The NSLS has developed the first global orbit feedback systems. These analog systems based upon harmonic analysis of the orbit motion reduced orbit fluctuations by more than an order of magnitude.
- Ongoing work is proceeding on the development of digital orbit feedback systems, allowing greater flexibility in the choice of algorithm, and hence further improvement in orbit stability.

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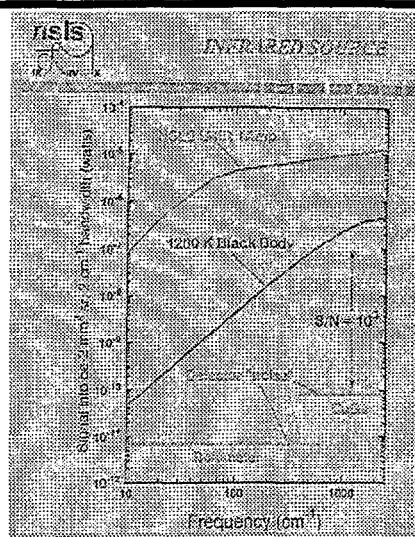
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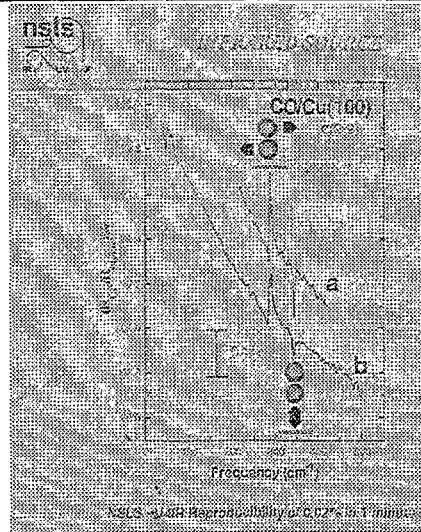




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SMALL GAP UNDULATOR MOTIVATION

$$B = B_0 \sin(Qz/\lambda)$$

$$B_0 = \mu_0 I_0 c / (G^2 \lambda)$$

$$I_0 = E_0 / 2c (4\pi K^2 C)$$

λ = undulator period

G = full gap

For short wavelength desire λ small

To high intensity desire $K = 0.93$ (A/T² A/cm)⁻¹

For high field strength short period requires

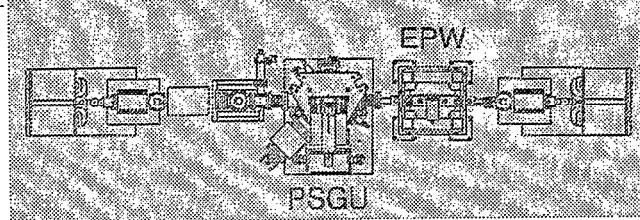
small gap

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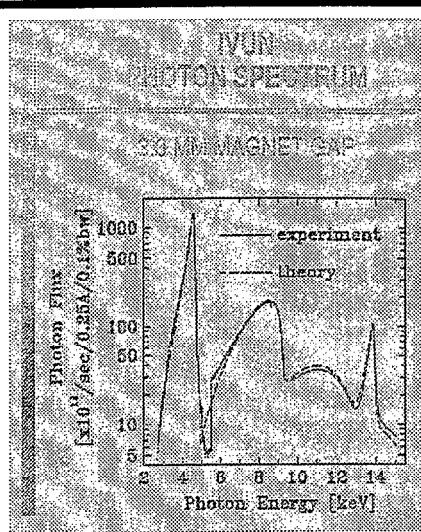
X13 R&D STRAIGHT SECTION



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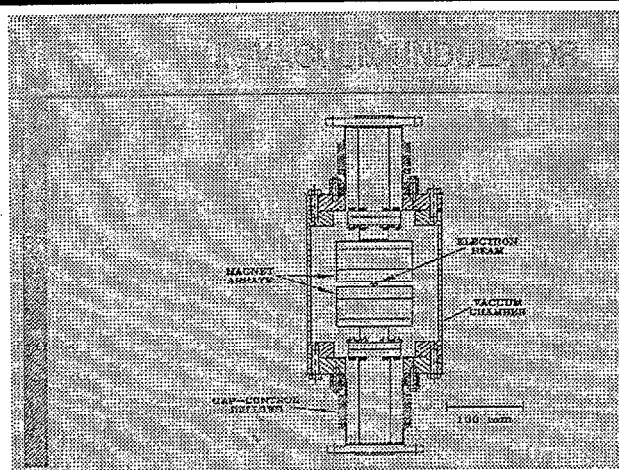
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NEW IVUNs AT X9 AND X29

- When we replace the RF Cavities at X9 and X29, we will install In-Vacuum Undulators at the center of the straights.
- These undulators will be of hybrid design, achieving higher fields than the pure permanent magnet devices tested in the X13 straight.

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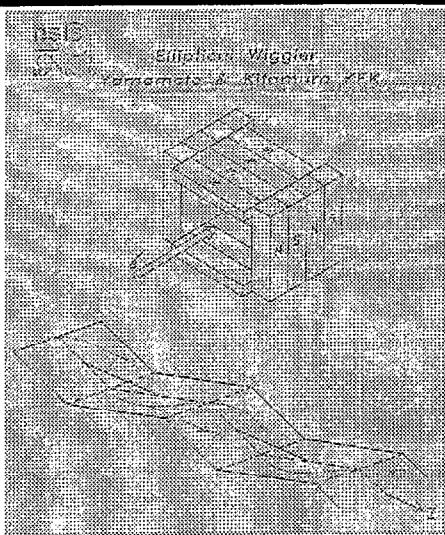


| | PSGM | IVUN | HYBRID IVUN |
|------------------------------|---------|---------|----------------|
| Period λ | 6 mm | 11 mm | 12.5 mm |
| Nominal Magnetic Gap | 6.0 mm | 3.3 mm | 3 mm |
| Beam Aperture | 3.0 mm | 3.0 mm | 3.0 mm |
| Peak On Axis Field b/T | 0.62 T | 0.68 T | 1.0 T |
| Electron Energy | 3.2 keV | 5.4 keV | 3.6 keV |
| | 2.8 GeV | 2.8 GeV | 2.8 GeV |

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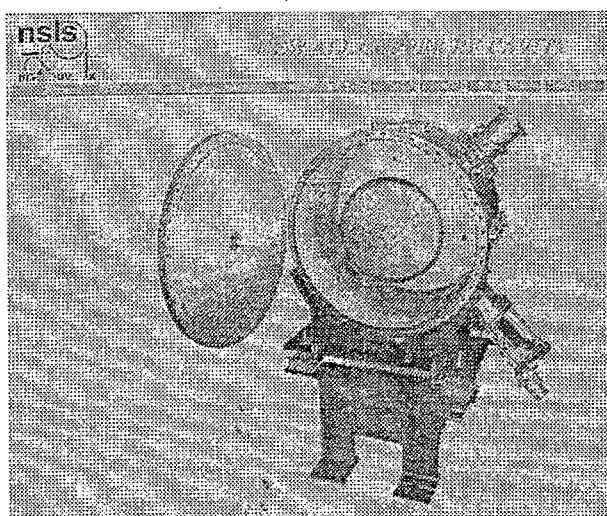




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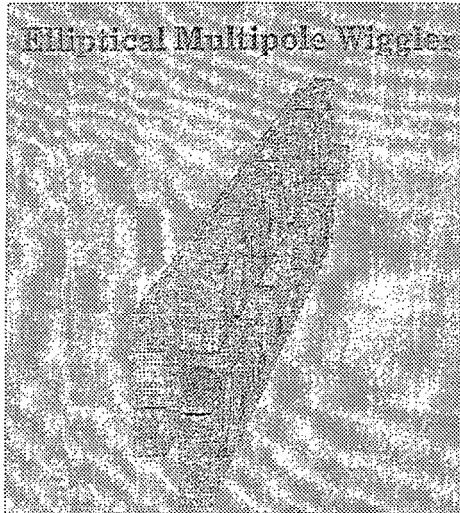
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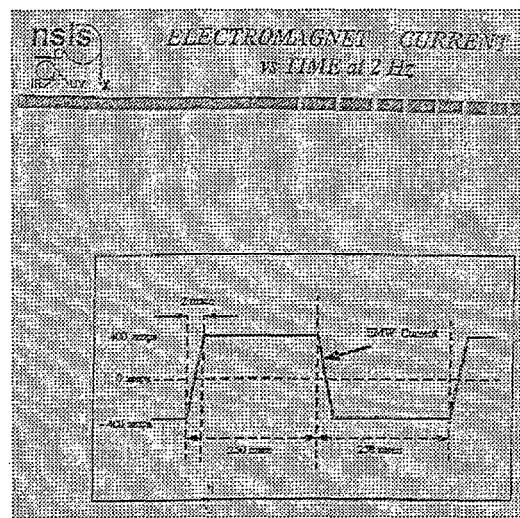
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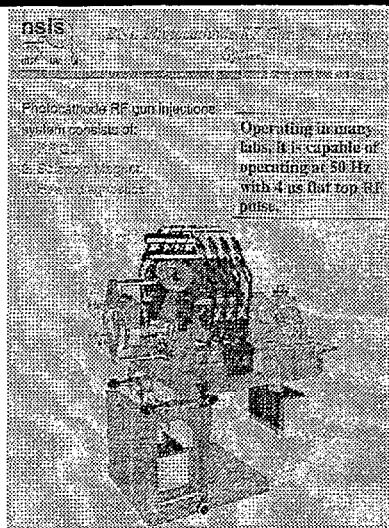
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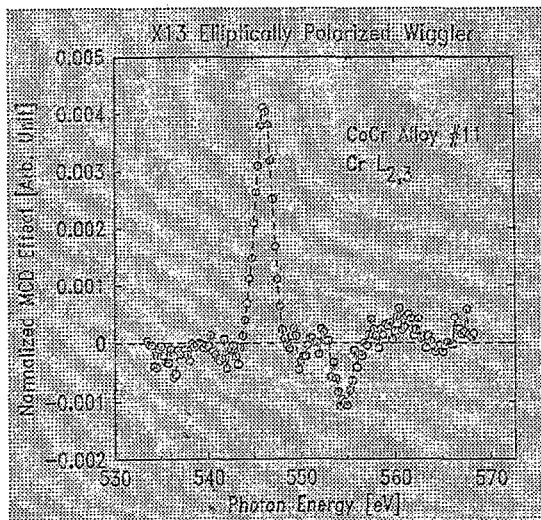
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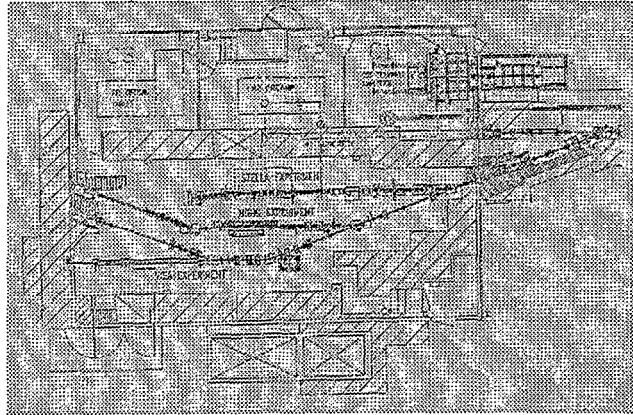
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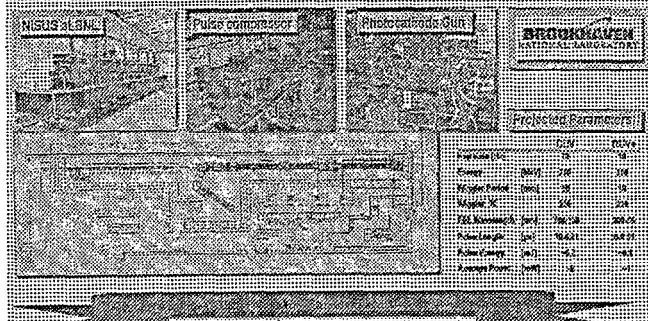
The Deep Ultra-Violet FEL

Brookhaven National Laboratory, Upton, New York 11973 USA

THE DUV-FEL is a dedicated platform for the development of a new class of FEL Technology and Science.

The only short wavelength FEL project based on Laser Seeded High Gain Harmonic Generation.

Many collaborative institutions: SLAC, APS, SLAC-LCLS, TUM & FEL, Ohio University, Maryland



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“NSLS Compared to the World”

Steven Hulbert

NSLS compared to "the world"

1. Introduction, SR emission properties of bends, wigglers, undulators
2. Flux
3. Brightness
4. Effect of brightness on three specific techniques (all using undulators)
 - A. High res'n angle-resolved photoemission
 - B. Zone-plate-based soft x-ray μ scopy
 - C. Hard x-ray microprobe

S. Hulbert, 23 October 2000

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Synchrotron radiation properties relevant to flux and brightness

Bend radius r , Energy E , critical energy E_{crit} , E/E_{crit}

| Machine | E [GeV] | γ | r [m] | B [T] | E/E_{crit} |
|------------|-----------|----------|---------|---------|--------------|
| NSLS (VME) | 0.8 | 1666 | 1.91 | 1.276 | 0.5911 |
| | 1.8 | 5197 | 3.875 | 1.278 | 1.08 |
| NSLS | 1.9 | 5718 | 4.81 | 1.317 | > 1.6 |
| ATLAS | 4.0 | 13400 | 32.96 | 0.6 | 17.5 |
| SEMARK | 3.0 | 5841 | 2.40 | 6.2 | 3.12 |

Insertion devices
N S N S
S N S N

period length λ_u , magnetic strength $K \sim \lambda_u B$

$$\# \text{ periods } N_u \quad \lambda_u = \frac{d_u}{2\pi} \left(1 + \frac{p^2}{2} + \frac{1}{2} \theta^2 \right)$$

Opening angles: Bend Wiggler Undulator

$$\begin{array}{lll} \text{Hori: } & \beta_p & 2K/\gamma \\ \text{Vert: } & 1/\gamma & 1/\alpha \end{array} \quad \sqrt{\lambda_u/L} \odot \text{beam}$$

Undulator Brightness, Flux

$$B = \frac{F}{(2\pi)^2 \lambda_u^2 L^2} \quad F = \frac{4\pi \alpha \beta_p}{\gamma^2} \quad \lambda_u = \frac{d_u}{2\pi} \left(1 + \frac{p^2}{2} + \frac{1}{2} \theta^2 \right)$$

$$\text{For point source, } B = F / (\lambda_u L)^2$$

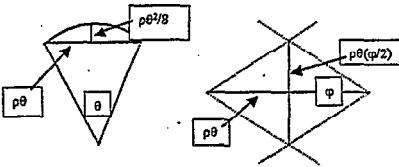
Diffraction Limited Brightness for Constant Field SR

$$\text{Flux integrated over all} = 5.3 \times 10^{17} E(\text{GeV}) I(\text{Amp}) \theta_{\text{full}}[\text{rad}] \text{BW}[\%] \left(\frac{\omega}{\omega_c} \right)^{1/3}$$

Vertical angles [ph/sec]

$$\text{RMS vertical opening angle: } \psi_{\text{rms}}^{1/2} = 0.8282 \left(\frac{\lambda}{2\pi\rho} \right)^{1/3}$$

$$\text{Phase Space Areas: Horizontal} = \frac{\rho\theta^2}{8} \theta \quad \text{Vertical} = \frac{\rho\theta\psi}{2} \psi$$



$$\text{Flux} \\ \text{Brightness: } B = \frac{\text{Phase.Space.vert.} \times \text{Phase.Space.hor.}}{\text{Area}}$$

$$\text{Assuming, } \theta = \psi = 4\psi_{\text{rms}}^{1/2}$$

$$B[\text{Photons/sec/0.1\%BW/mm}^2/\text{steradian}] = 3.8 \times 10^{-6} \frac{\text{BW}[\%] I[\text{Amp}]}{\lambda^2 \text{mm}}$$

Jim Murphy, NSLS

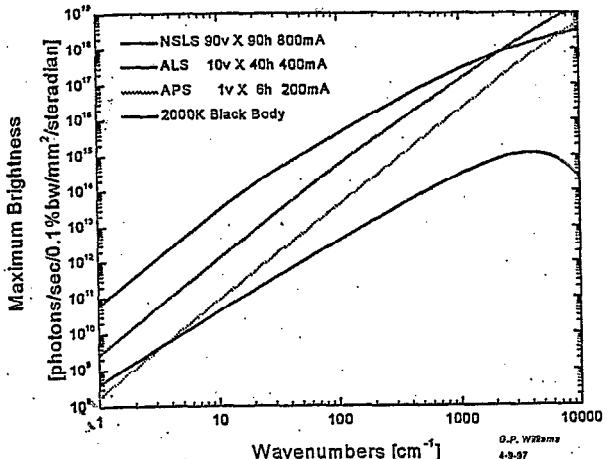
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Features of Synchrotron Infrared

- High brightness source:
>2 orders of magnitude brighter than standard source for IR
 - enables study of small specimens and at long wavelengths.
microspectroscopy
- Pulsed: enables time-resolved measurements across wide spectral range.
 - *pump-probe spectroscopy*
 - ~200 ps resolution

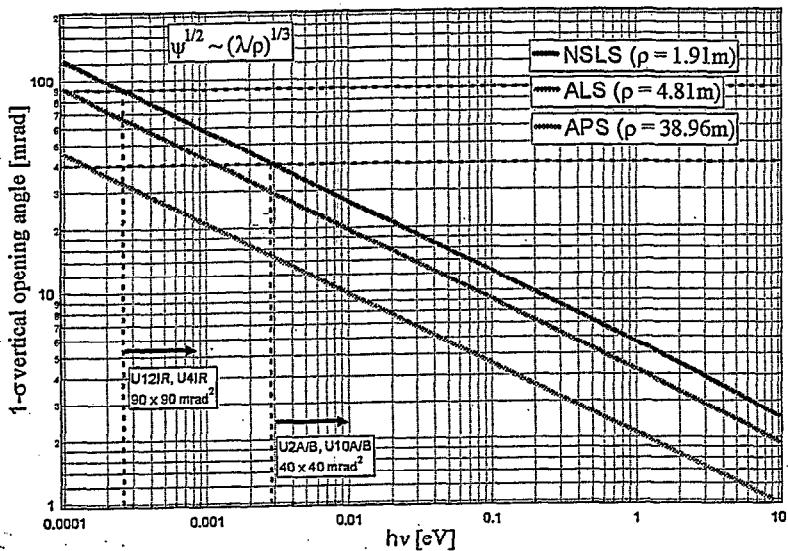


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Synchrotron radiation vertical opening angles in the infrared

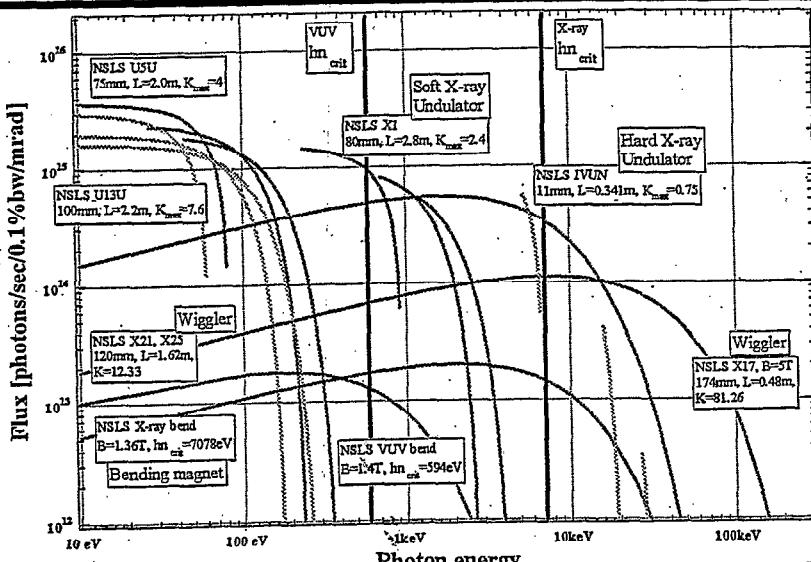


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Flux of NSLS today (2.8GeV,0.32A)

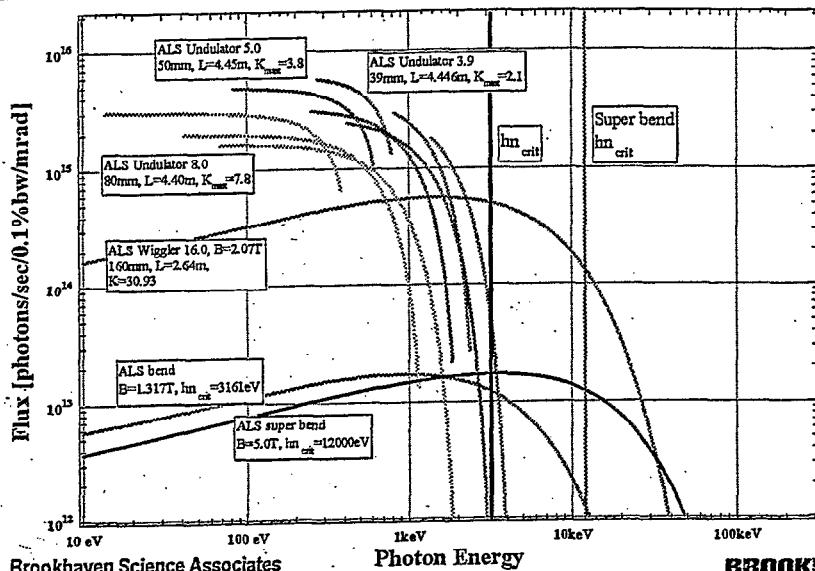


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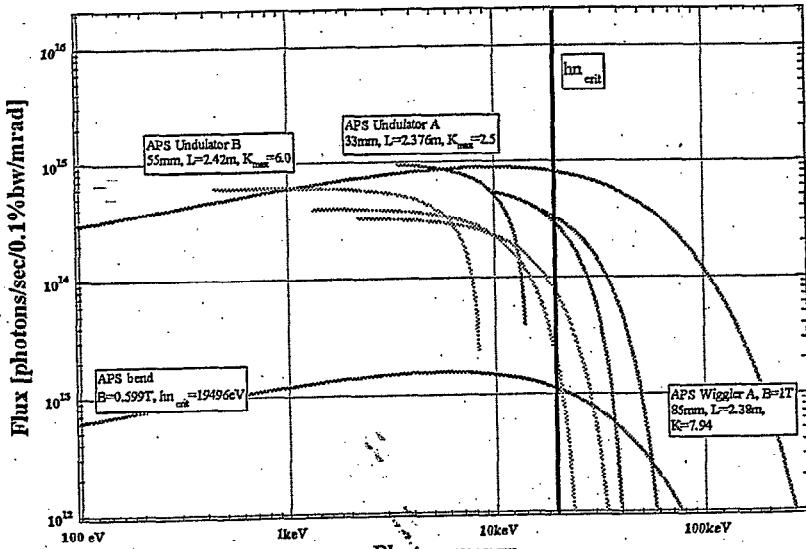
ALS flux (0.4A)



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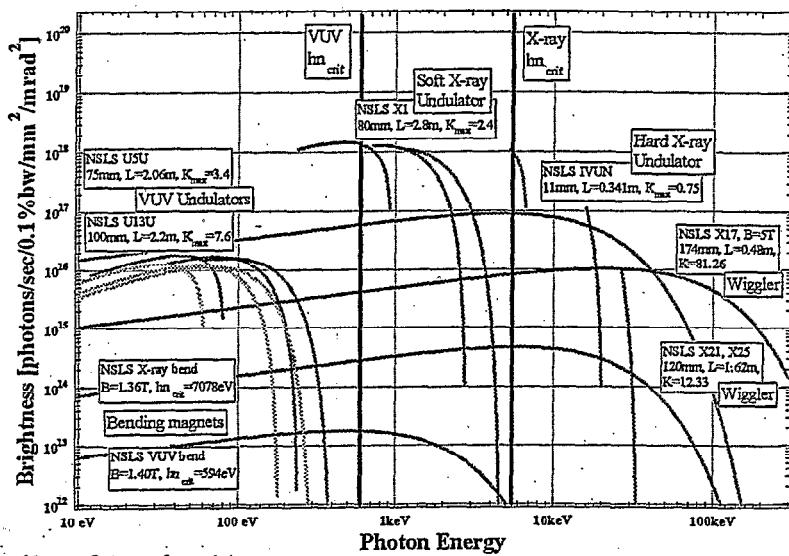
APS flux (0.1A)



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Brightness of NSLS today

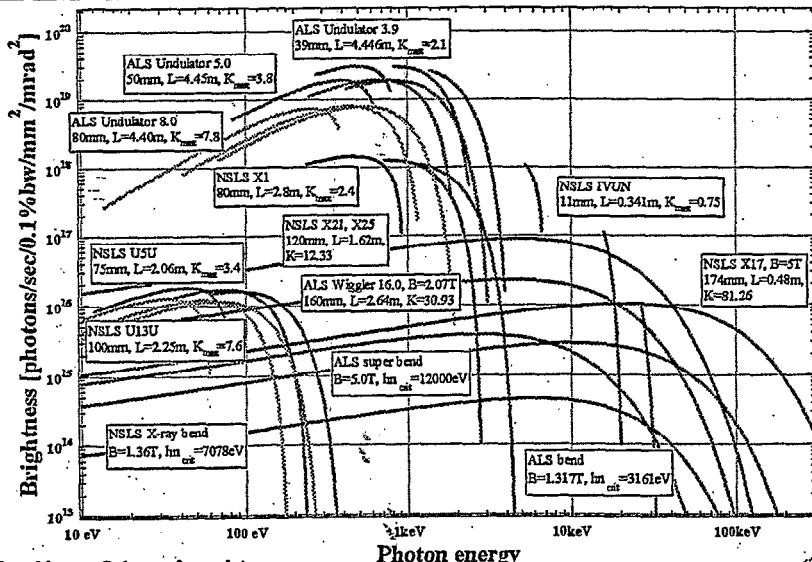


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Brightness comparison: NSLS (0.32A) vs. ALS (0.4A)

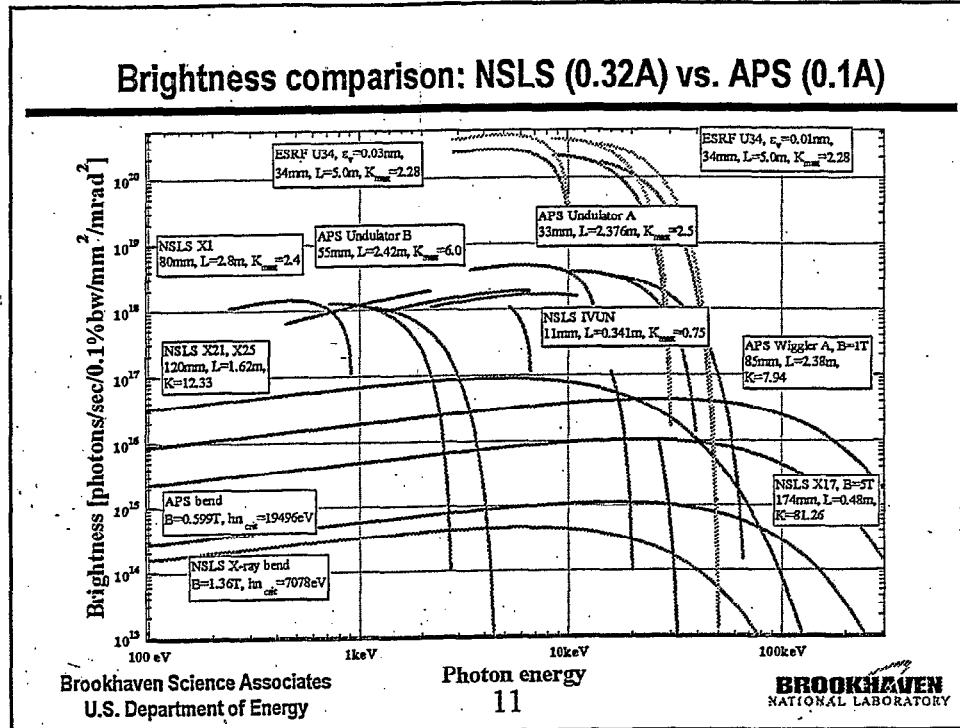


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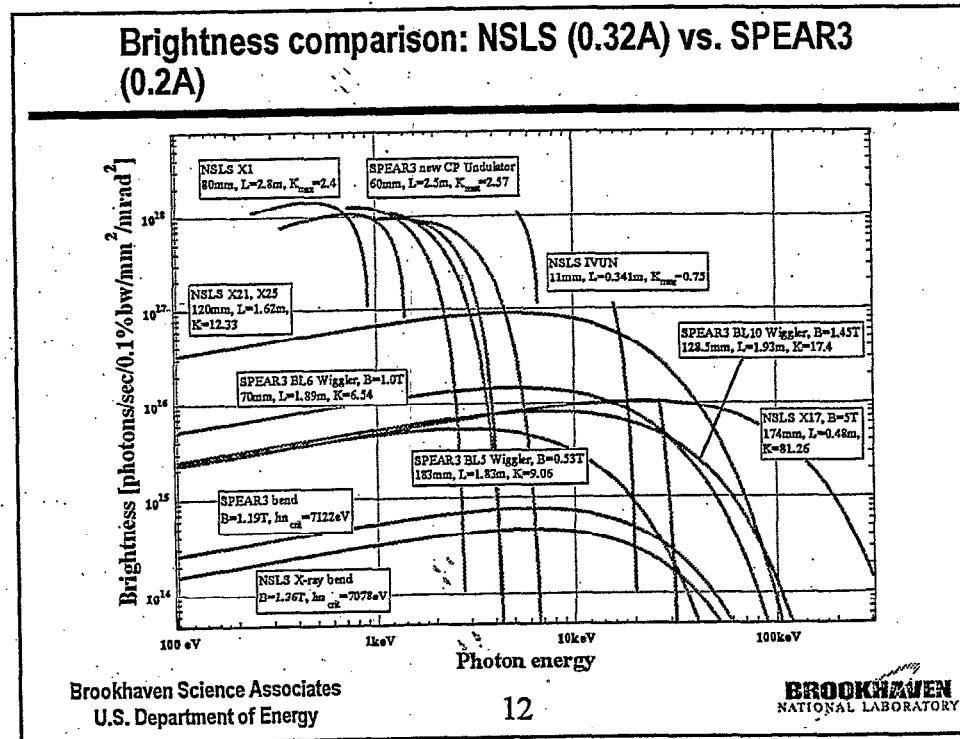
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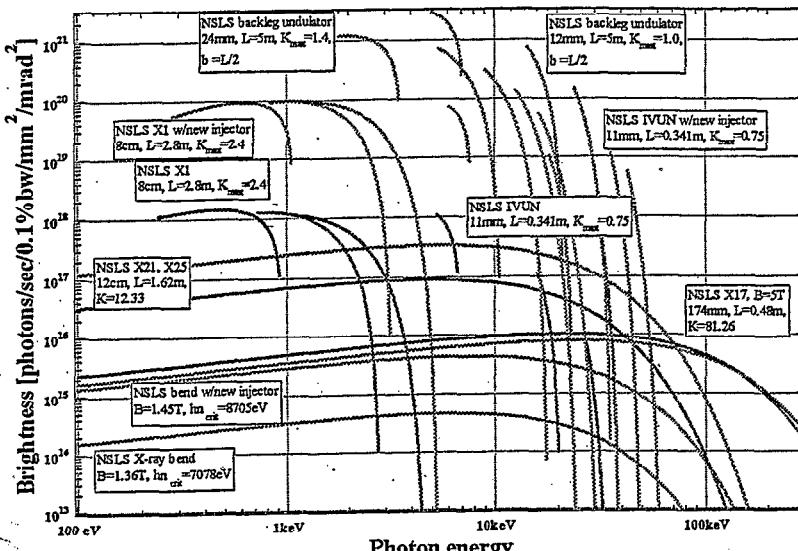
Brightness comparison: NSLS (0.32A) vs. APS (0.1A)



Brightness comparison: NSLS (0.32A) vs. SPEAR3 (0.2A)



Brightness comparison: NSLS today (0.32Å) vs. new linac injector (0.2Å)



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C-PLOT Graphics
Creator:
C-PLOT postscript version 4.13
Preview:
This EPS picture was not saved
with a preview included in it.
Comment:
This EPS picture will print to a
PostScript printer, but not to
other types of printers.

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NSLS U13UB 5-30eV beamline: high-resolution ARPES

Normal incidence monochromator (NIM), resolving power $> 10^4$
Flux at sample: $> 3 \times 10^{13}$ photons/sec/A/0.1%bw. into <100micron spot size
Undulator brightness: $> 10^{16}$ photons/sec/A/mm²/mrad²/0.1%bw.

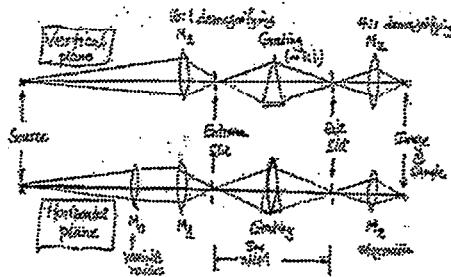
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Creator: AutoCAD PSOUT
CreationDate: 1997-05-08

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NSLS U13UB VUV undulator and NIM beamline: matching source to experiment



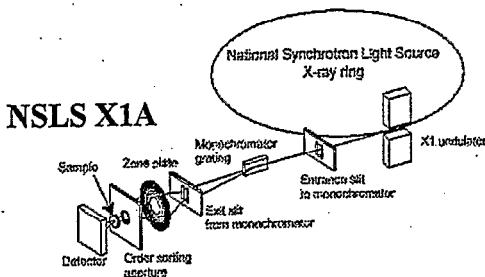
- demagnify source vertically to fill enough lines ($\lambda/\Delta\omega > 5\pi^2$) for dispersion
- total demagnification $\sim 64:1$ in both horizontal and vertical $\Rightarrow 0.1 \text{ mm}^2$ spot size on sample
- achieves state-of-the-art
- Electron gun
- electron energy analyzer (EEA)

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NSLS X1A: soft x-ray scanning microscopy



- Zone plate accepts only $\sim \lambda$ transverse phase space.
- This acceptance is $\sim 100\%$ vertically, but only $\sim 1\%$ horizontally.
- Brightness and count rates of X1A are ~ 0.1 of 3rd generation:
 - X1A can still perform very well, but
 - NSLS needs greater brightness undulators in the soft x-ray range.

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Transverse spatial coherence of SR sources

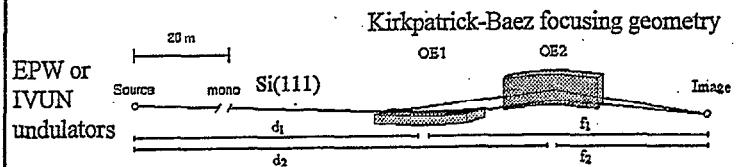
Title: C-PLOT Graphics
Creator: C-PLOT pattern version 4.13
Format: EPS
This EPS picture was not saved with a preview included in it.
Comment: This EPS picture will print to a PostScript printer, but not to other types of printers.

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X-ray μprobe using differentially-coated elliptical mirrors*

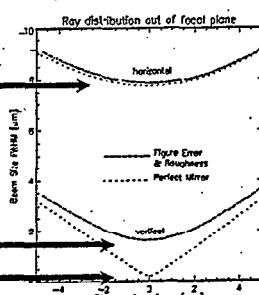


Focus limitations:

1. Large Horizontal emittance

2. Mirror figure error

Perfect ellipsoid



■ Flux limitation: overfilling of horizontal mirror (OE2). Cannot make OE2 larger without interfering with OE1 or experimental endstation

*Beamlime Technology Corp.; R&D 100 Award, Sept. 2000

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Worldwide compendium of x-ray μprobes

Gene Ice, ORNL

| Facility | Beamline | Inv. μJ/eV | Spot size μm ² | Δλ/λ | Total Flux ph/sr/Å ² | Local Contact | Email |
|----------|----------|---------------|------------------------------|---------------------------|--|--------------------|---------------------------|
| ALS | 2-00-CD | ~4.25 | ~4 | 2x10 ⁻⁴ | 3x10 ²⁴ | Wen-Bing Yau | Yau@aps.anl.gov |
| ALS | 3B-23 | ~2.25 | ~5 | 2x10 ⁻⁴ | 3x10 ²⁴ | Steve Sotomayor | Sotomayor@aps.anl.gov |
| NSLS | 3D-33 | ~3.15 | ~6.5 | 2x10 ⁻⁴ | 3x10 ²⁴ | Christian Wickert | wickert@nsrl.sfa.edu |
| ESRF | ID-12 | ~3.55 | ~3 | 2x10 ⁻⁴ | 10 ²⁴ -10 ²⁵ | Agnieszka Szarejko | szarejko@esrf.fr |
| ALS | 6G-3.1 | 6.12 | ~2 | 3x10 ⁻³ | 2x10 ²⁴ | Steve McHugh | smcmh@cds.ornl.gov |
| LNLS | | 2.14 | 400 | 2x10 ⁻⁴ | 3x10 ²⁴ | Heiko Uhl | uhl@esrf.fr |
| CATRIS | IR | ~3.5 | 0.801 | 2x10 ⁻⁴ | 10 ²⁴ | Dan Alderback | dan@esrf.esrf.fr |
| ESRF | SHINE | ~4.13 | 25 | 2x10 ⁻⁴ | 10 ²⁴ | A. Iida | |
| HASYlab | L | ~4.00 | ~4 | | | Thomas Stroblowski | stroblowski@fz-juelich.de |
| HASYlab | BW-1 | 10 | ~4 | 4x10 ⁻⁴ | 4x10 ²⁴ | Thomas Stroblowski | stroblowski@fz-juelich.de |
| DCX | DHS | 5.16 | ~4-100 | 2x10 ⁻⁴ | 10 ²⁴ -10 ²⁵ | P. Chavallier | chavallier@impmn.cea.fr |
| SSRL | | | | | | P. Patel | patel@slac.stanford.edu |
| NSLS | X10AC | 5.25 | ~400 ^a | White | 10 ²⁴ | M. Marcus | |
| NSLS | X10A | 5.25 | ~45 ^a 2nd beam | 10 ²⁴ white | 2x10 ²⁴ 2x10 ²⁴ | Steve Sotomayor | Sotomayor@aps.anl.gov |
| NSLS | X13B | 4.22 | 3x9μm ² | 10 ⁴ | 3x10 ²⁴ | C.C.Kao/J. Ablett | kao@bnl.gov |
| IVUN | | | | | | | |

→ Need higher brightness x-ray undulators at NSLS

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Summary: NSLS vs. "the world"

| | Far-IR spectroscopy | VUV spectroscopy | Soft x-ray μscopy | Hard x-ray μscopy |
|---------------------|--|--|---|--|
| Brightness ratio | > 3 rd gen. SR | ~0.1 × 3 rd gen. SR | ~0.1 × 3 rd gen. SR | ~0.01 × 3 rd gen. SR |
| Count rate ratio | > 3 rd gen. SR | ~1 × 3 rd gen. SR | ~0.1 × 3 rd gen. SR | ~0.01 × 3 rd gen. SR |
| | Want shorter pulses for spectroscopy and smaller emittance for μscopy | Want shorter pulses for spectroscopy and smaller emittance for μscopy | Want smaller emittance (by factor ≥10) 3GeV source | Want smaller emittance (by factor ≥100) 6GeV source |

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“Science with Synchrotron Radiation”

Chi-Chang Kao

Science with Synchrotron Radiation

-Highlights from NSLS

Prepared by Chi-Chang Kao.

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NSLS Users by Field of Research (1990-2000)

Number of Users

1200
1000
800
600
400
200
0

| Type of Science | 1990 | 1991 | 1992 | 1993 | 1994 | 1995 | 1996 | 1997 | 1998 | 1999 | 2000 |
|---------------------------------|------|------|------|------|------|------|------|------|------|------|------|
| Chemical Sciences | 264 | 304 | 303 | 318 | 321 | 281 | 292 | 285 | 268 | 265 | 244 |
| Materials Sciences | 837 | 993 | 882 | 1104 | 929 | 952 | 916 | 902 | 914 | 819 | 842 |
| Life Sciences | 62 | 167 | 206 | 354 | 503 | 548 | 642 | 701 | 761 | 881 | 953 |
| Geosciences and Ecology | 62 | 26 | 75 | 80 | 113 | 106 | 123 | 136 | 147 | 147 | 177 |
| Applied Science and Engineering | 155 | 106 | 167 | 186 | 177 | 147 | 138 | 126 | 127 | 134 | 119 |
| Optical/Nuclear/General Physics | 170 | 129 | 183 | 151 | 129 | 128 | 116 | 136 | 131 | 138 | 162 |
| None Specified | 0 | 0 | 1 | 0 | 56 | 44 | 34 | 34 | 32 | 32 | 54 |
| Total | 1550 | 1725 | 1897 | 2193 | 2228 | 2206 | 2261 | 2320 | 2380 | 2416 | 2551 |

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NSLS leads the world in scientific productivity

**BESAC Review of SR Sources and Science
"Birgeneau Report" – Spring, 1997**

BESAC Review of ALS – March 29, 2000

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Birgeneau Report / 1990-1996

| Nature | Science | Phys. Rev. Lett. |
|----------|----------|------------------|
| NSLS: 51 | NSLS: 55 | NSLS: 234 |
| SSRL: 17 | SSRL: 27 | SSRL: 49 |

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*NSLS 1997 – 1999 Publications in
Nature, Science and Physical Review Letters*

| 1997 | 1998 | 1999 |
|----------------------------|---------------------------|--------------------------|
| Science: 16 (B10,G4,P1) | Science: 15 (B11,G4) | Science: 8 (B4,G3,P1) |
| Nature: 8 (B6,G1,P1) | Nature: 16 (B13,G2,P1) | Nature: 7 (B4,G1,P2) |
| Phys.Rev.Lett:19 | Phys.Rev.Lett:18 | Phys.Rev.Lett:18 |

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NSLS leads the world in scientific productivity

- The spectral range covered by the NSLS extends from far-infrared (1 meV) to gamma-ray (100 keV)
- Innovation and improvement in source and technique
- A large and diverse user base
- Intangibles: stimulating environment, flexibility

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Scientific Opportunities of Proposed Upgrades

Flux: Lonny Berman
(Protein Crystallography)

Brightness: Erik Johnson

Short Pulse + FEL: Jerry Hastings

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Life Sciences

-Protein Crystallography

-Non PX Biological Research
(spectroscopy, imaging, scattering)

-Medical imaging

-Radiation Therapy

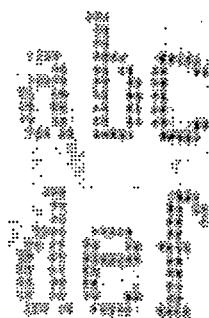
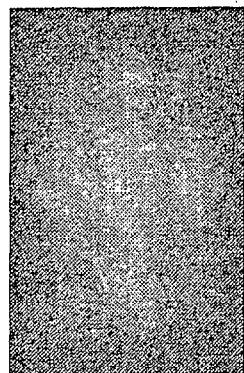
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Extending X-ray Crystallography to Non-Crystalline Samples

J. Miao, P. Charalambous, J. Kirz, D. Sayre, Nature 400, 342 (1999)

X-ray scattering using Coherent X-rays

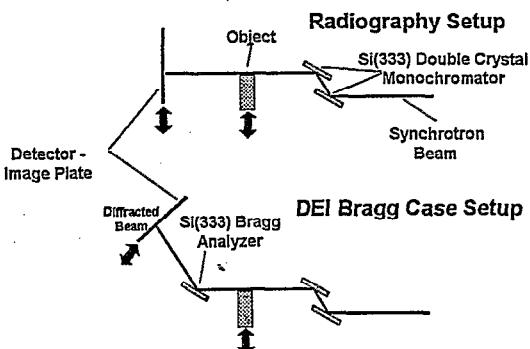


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Diffraction Enhanced Imaging at NSLS-X15A

**DEI --- Normal Absorption
Refraction; Extinction -or- Scatter Rejection**



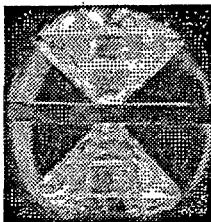
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Geophysics and High Pressure

*If you can't bring the synchrotron to your laboratory,
bring the laboratory to the synchrotron.*

Infrared



Energy Dispersive Diffraction

P as an experimental variable can
be exploited in solid state physics,
materials synthesis, life science.

X-ray Spectroscopy

**Center for High Pressure Research – SUNY Stony Brook
Geophysical Laboratory of the Carnegie Institution of Washington**

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Correlated Electron Systems

- Low-dimensional, Strongly Correlated Electron Systems Exhibit Non-Fermi Liquid Behaviors
- Coupling of Charge, Spin, and Orbital D.O.F

Infrared



Theory

Photoemission

Samples

X-ray Absorption

Technology

Resonant X-ray Scattering

Transport measurements

Inelastic X-ray Scattering

Other Techniques: NMR,
Neutron, TEM, STM etc.

Coherent X-ray Scattering

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New Directions

Nanoscience

(workshop/Dec. 2000)

Soft Condensed Matters/Biophysics

(workshop/early 2001)

***In-Situ* growth and characterization**

(workshop/planning)

Environmental Science

(workshop/planning)

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Infrared Measurements

Need:

- High brightness continuum IR source (especially in far IR) for throughput-limited spectroscopic techniques.
- Broad spectral coverage for sum rules, K-K analysis.
- Short pulses for time-resolved techniques (ps, fs).
- Quasi-tunable, higher power far IR source for photo-excitation & study of non-linear phenomena.

NSLS provides:

- ❖ Two to three orders of magnitude higher brightness than thermal sources: exploited for microspectroscopy, grazing incidence reflectance, ellipsometry. Good far IR power (up to 2 orders of magnitude higher than thermal sources).
- ❖ Complete IR spectral coverage.
- ❖ Pulses widths down to ~200 ps.

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Infrared Measurements

Future?:

- ◆ Shorter pulses (time-resolution)
- ◆ Even greater brightness (for near-field microscopy)
- ◆ Coherent far IR source

Recent Infrared Publications

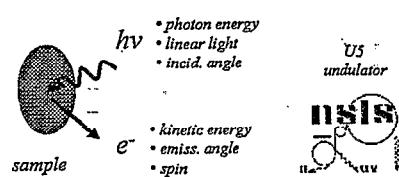
- G.L. Carr et al., "Exploring the dynamics of superconductors by time-resolved far-infrared spectroscopy", *Phys. Rev. Lett.* **85**, 3001 (2000).
- A.A. Sirenko et al., "Soft-mode hardening in SrTiO₃ thin films", *Nature* **404**, 373 (2000).
- P.F. Henning et al., "Infrared studies of the onset of conductivity in ultrathin Pb films", *Phys. Rev. Lett.*, **83** (1999).

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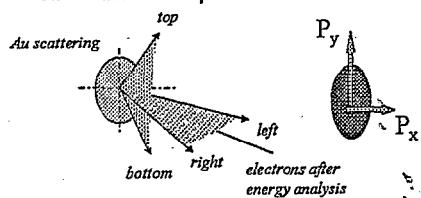


Spin-Resolved Photoemission U5UA (10-200 eV)

Experimental Technique

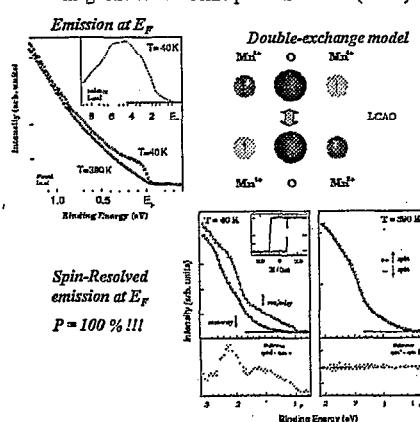


Two-dimensional Spin Detector



Manganites $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$

magnetic & electronic phase transition (CMR)



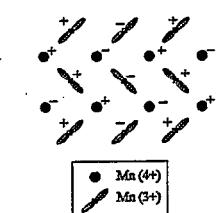
J.-H. Park et al., *Nature* **392**, 794 (1998)

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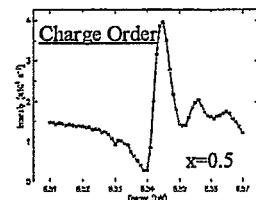
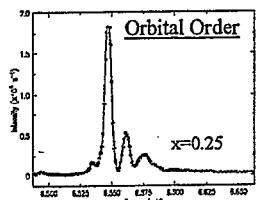
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Resonant scattering from Spin, Orbital and Charge Order in Transition Metal Oxides

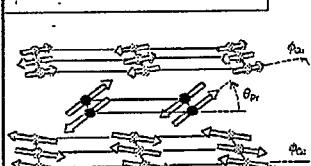
Manganites



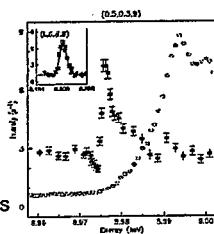
Resonant scattering at Mn K-edge



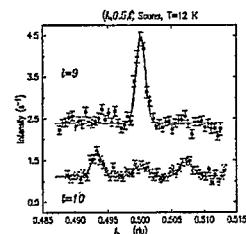
Cuprates



Magnetic scattering at Cu K-edge



ESRF
data



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“Improvements to Existing Facility”

D. Peter Siddons

Improvements to Existing Facility

What could be done to the status quo which would result in significant benefit to the User community and to the Laboratory?

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Two main aspects

- Infrastructure improvements
- New access paradigm

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Infrastructure Improvements

- Replacing old beamline hardware.
- Replacing old machine hardware (including insertion devices).
- Providing better User Facilities.

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3



Update old beamline hardware

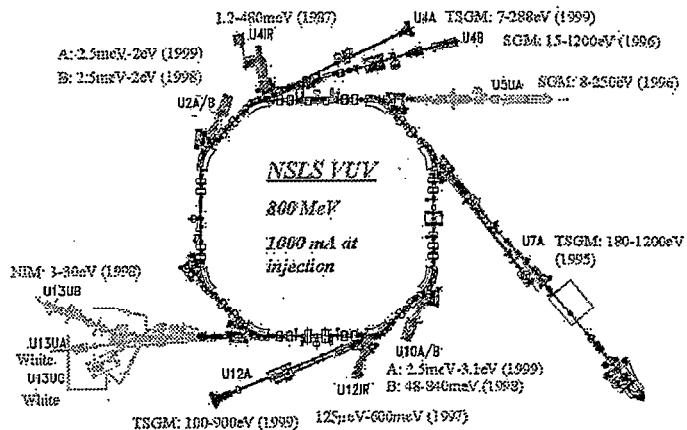
- Much of the hardware dates from 1985. (at least two beamlines still rely on MicroVax for control, for example).
- Mirror technology has improved dramatically since 1985.
- Power delivered to optics has increased by factor of 10 since then; inefficient monochromators.

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VUV ring beamline upgrades



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Update old Machine Hardware

- Much has been and is being replaced on a continuous basis (e.g. RF cavities, power supplies).
- This is all covered in detail in the Phase III proposal. Most of the things in that report are still relevant (or have been done already).
- Our original Insertion devices were designed over 10 years ago. Better designs now exist, and optimization for our needs would likely yield improvements of x2 - x5 in performance.

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Increased efficiency from mirror upgrade

TIME
C-PLOT Graphics
1 C-PLOT printer version 4.13
Preview:
This EPS picture was not saved
with a preview included in it.
Comments:
This EPS picture will print to a
PostScript printer, but not to
other types of printers.

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Providing better User Facilities

- Lab facilities.
 - Sample preparation equipment,
 - standard characterization tools and
 - Staff to maintain/operate them.

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A New Access Paradigm for NSLS

- Current system has served NSLS well, but is inappropriate for today's situation
 - Difficult to generate funding for a single-technique beamline over extended periods.
 - New users are NOT technique-developers.
 - E.g. the VUV beamlines almost all rebuilt by NSLS, not PRT's.
- Emphasis must shift from technique development to scientific productivity.
 - Most problems benefit from a multi-pronged investigation.
 - Multi-PRT membership is prohibitively expensive.
 - It is difficult to get GU beamtime for a measurement which is a small, but important part of a larger investigation.
 - Multi-function beamlines don't work well.

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PRT operations support

- PRTs initially supported NSLS beamlines at a high level, typically two scientists per beamline plus a technical staff.
- Currently, typical PRT staffing is one scientist per beamline, sometimes with one technician.
- NSLS cannot replace this support with current funding.

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Science-centered organization

- Deterministic access to all techniques appropriate to the scientific problem.
- Expert assistance at each stage:
 - Experiment design
 - Data collection
 - Data interpretation

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Straw-man example: Materials Growth & Characterization

- Techniques set:
 - Spectroscopy:
 - IR
 - VUV
 - X-ray
 - Scattering/diffraction:
 - N-circle diffractometer
 - Powder diffractometer
 - SAXS
 - Imaging:
 - IR microscope
 - VUV/SXR scanning microscope
 - XMCT

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Science / technique matrix

| | Soft X-ray Scanning Microscopy | X-ray Microscopy | X-ray Microtopography | X-ray Microscopy | IMAGING | SPECTROSCOPY | POLARIZATION | Single Crystal Diffraction | Small Angle X-ray Scattering | DIFFRACTION SCATTERING |
|---|--------------------------------|------------------|-----------------------|------------------|---------|--------------|--------------|----------------------------|------------------------------|------------------------|
| ENVIRONMENTAL & MOLECULAR SCIENCES | | | | | | | | | | |
| Remediation | | | | | | | | | | |
| Proteins and Enzymes | | | | | | | | | | |
| COMPLEX SYSTEMS | | | | | | | | | | |
| Correlated Electron Systems | | | | | | | | | | |
| Soft Matter/Biophysics | | | | | | | | | | |
| EARTH & PLANETARY SCIENCE | | | | | | | | | | |
| NANOSCIENCE TECHNOLOGY | | | | | | | | | | |
| Materal Growth and Characterization | | | | | | | | | | |
| Materials Components for Electronic Devices | | | | | | | | | | |

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Staffing levels at other light sources

- ESRF
 - 2 scientists
 - 2 postdocs
 - 1 student (funded by ESRF, more with external funding)
 - Facility infrastructure (computers, electronics, mechanical engineering)
- APS DND-CAT
 - 8 staff / 2 beamlines. PRT member-funded students/postdocs.
- ALS
 - No public info, but \$7M provides GU support on 25 beamlines (~ 2 persons per beamline?).

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Current NSLS-operated beamline staffing levels

- X27A 1 Science Associate
- X18B 1 Science Associate
- X19A 1 Scientist
- X21 0.5 Scientist, 1 student
- U5U 1 Scientist, 1 student
-

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Current PRT-operated beamline resident staffing levels

- X11 1 Scientist, 1 technician
- X16A,B,C 1 technician
- X3A,B,C 1 Scientist, various students.
- X8A 1 Scientist
- X10A,B,C1 Engineer
- X14 1 Postdoc
-

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Upgrade Options to be Discussed:

“Increase Current in X-ray Ring Using B-Factory Technology B-Factory Upgrade, Accelerator”

Eric Blum

X-RAY RING UPGRADE USING B-FACTORY TECHNOLOGY

**ERIC B. BLUM
NATIONAL SYNCHROTRON LIGHT SOURCE
OCTOBER 23, 2000**

Upgrade Goals

- Energy — 3 GeV
- Current — 2.4 Amp

Means

- 476 MHz RF — Room Temperature Cavities
- Copper Vacuum Chamber
- Bunch by Bunch Feedback
- Full Energy Injection

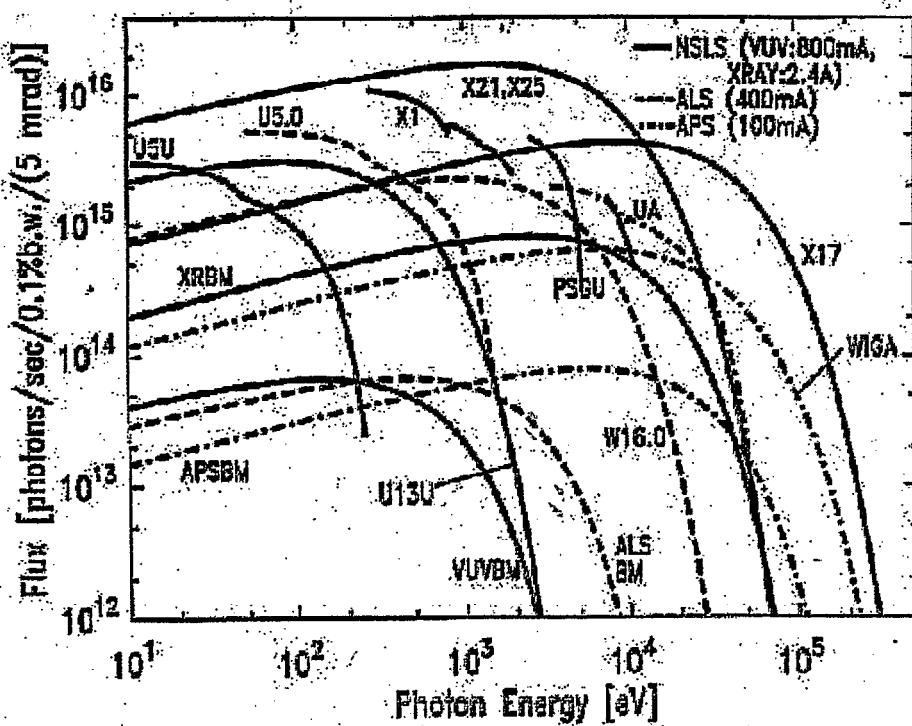
PEP-II Low Energy Ring

- Energy — 3.1 GeV
- Current — 3.0 Amp maximum

Means

- 476 MHz RF — Room Temperature Cavities
- Copper Vacuum Chamber
- Bunch by Bunch Feedback
- Full Energy Injection

FLUX AT UPGRADED NSLS, ALS, AND APS



MAJOR X-RAY RING PARAMETERS

| | Current Conditions | Upgrade with single RF system | Upgrade with harmonic cavity |
|--|-----------------------|----------------------------------|---------------------------------|
| Energy [GeV] | 2.5 | 3 | 3 |
| Total Current [A] | 0.25 | 2.42 | 2.42 |
| Fund. Cavity RF Frequency [MHz] | 52.88 | 475.92 | 475.92 |
| Fund. Cavity RF peak voltage [MV] | 0.9 | 4.27 | 4.26 |
| RF harmonic | 30 | 270 | 270 |
| Number of Bunches Filled | 25 | 225 | 225 |
| Harmonic Cavity RF Frequency [MHz] | | | 951.84 |
| Harmonic Cavity RF peak voltage [MV] | | | 2.04 |
| Bunch Length [cm] | 4.33 | 0.73 | 2.64 |
| Synch. Rad. Loss [MeV/turn] (bends only) | 0.50 | 1.04 | 1.04 |
| Transverse Damping Time [msec] | 219.15 | 378.69 | 378.69 |
| Longitudinal Damping Time [msec] | 438.30 | 757.39 | 757.39 |
| Energy Acceptance | 1.82% | 1.82% | 1.82% |
| Synch. Freq. [KHz] (fund. RF only) | 5.91 | 35.24 | 35.22 |
| Touschek lifetime [hours] | 356 | 59 | 213 |

RF Cavity Choice:
Superconducting vs. Conventional

Superconducting Cavity

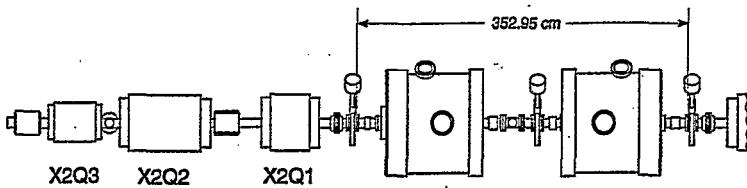
- Pro:**
- Large Gradients — Fewer Cavities
 - Lower RF Power Consumption
 - Large Aperture
 - Easy Higher Mode Removal —
 - Beam Instabilities Reduced

- Con:**
- Technology Less Used
 - No Experience at NSLS

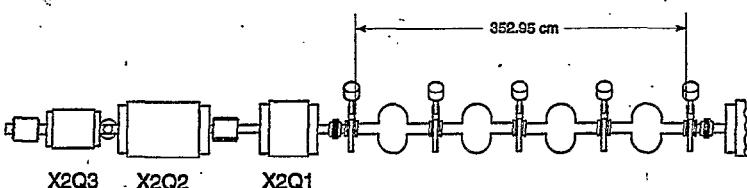
Conventional Cavity (Room Temperature Copper)

- Pro:**
- Common Technology
 - Simpler Fabrication
 - No Cryogenics
- Con:**
- More Cavities Required
 - Higher Modes — Beam Instabilities — Feedback

RF CAVITIES



Existing Configuration of X-Ray Ring showing 52.88 MHz RF cavities.



Possible Configuration with Four PEP II 476 MHz RF cavities.

476 MHz RF System Parameters

| | PEP-II | |
|--|--------|------|
| Frequency [MHz] | 475.92 | 476 |
| Peak Voltage [MV] | 4.26 | |
| Harmonic Number | 270 | |
| Synchrotron Radiation Loss [MeV/turn] (bends only) | 1.04 | |
| Synchronous Phase [Deg.] | 19.03 | |
| Number of Cavities | 8 | |
| Gap Voltage/Cavity [MV] | 0.53 | |
| Cavity Gap [cm] | 22.34 | |
| Gradient [MV/m] | 2.39 | 4.5 |
| Shunt Impedance/Cavity [$M\Omega$] | 3.50 | |
| Wall Loss/Cavity [KW] | 40.6 | 150 |
| Total Cavity Wall Loss [KW] | 325 | |
| Synchrotron Radiation Power [KW] | 2525 | |
| HOM Power [KW] | 417 | |
| Total Power Loss [KW] | 3266 | |
| Power Loss/Cavity [KW] | 298 | |
| Tuning Angle (deg) | 88.25 | |
| Reflected Power/Cavity [KW] | 4.26 | |
| Input Power/Cavity [KW] | 413 | 450 |
| Number of Klystrons | 4 | |
| Required Power/Klystron [KW] | 825 | 1200 |

HARMONIC CAVITY RF PARAMETERS

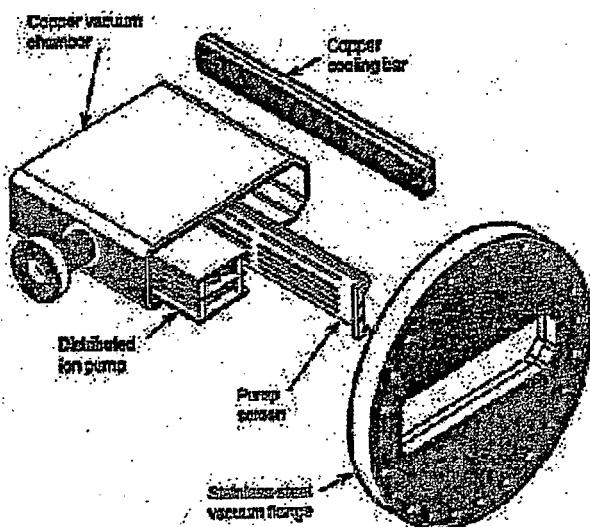
| | Valvo Klystron |
|--------------------------------------|-------------------|
| Frequency [MHz] | 951.84 |
| Peak Voltage [MV] | 2.04 |
| Synchronous Phase [Deg.] | 4.89 |
| Number of Cavities | 2 |
| Gap Voltage/Cavity [MV] | 1.02 |
| Cavity Gap [cm] | 11.17 |
| Gradient [MV/m] | 9.15 |
| Shunt Impedance/Cavity [$M\Omega$] | 4.95 |
| Wall Loss/Cavity [KW] | 106 |
| Total Cavity Wall Loss [KW] | 211 |
| Number of Klystrons | 1 |
| Required Power/Klystron [KW] | 211 400 |

Copper Vacuum Chambers

•10 Lower Photodesorption Than Aluminum

•Improved Thermal Conductivity

•Higher Z - Self Shielding



PEP B-Factory Chamber

SYNCHROTRON RADIATION LOADS

| | Current Conditions | Upgrade | PEP -II HER (Max. Current) |
|----------------------------------|-----------------------|---------|----------------------------------|
| Magnetic Radius [m] | 6.88 | 6.88 | 165.00 |
| Bending Magnet Field [T] | 1.21 | 1.45 | 0.182 |
| Energy [GeV] | 2.50 | 3.00 | 9.00 |
| Current [A] | 0.25 | 2.42 | 3.00 |
| Synchrotron Radiation Power [KW] | 125.71 | 2524.68 | 10,557 |
| Linear Power Density [W/cm] | 29.10 | 584.46 | 101.80 |
| Radiation Half Angle [mrad] | 0.20 | 0.17 | 0.06 |
| Chamber Width [cm] | 8.00 | 8.00 | 9.00 |
| Beam to Chamber Distance [cm] | 74.27 | 74.27 | 385 |
| Minimum Height Illuminated [mm] | 0.30 | 0.25 | 0.44 |
| Maximum Power Density [KW/cm^2] | 0.10 | 2.31 | 2.31 |

VACUUM LOADS

| | Current Conditions | Upgrade |
|---|-----------------------|----------|
| Material | Al | Cu |
| Desorption Coefficient η | 4.00E-06 | 4.00E-07 |
| Photodesorption Gas Load Q [Torr-L/sec] | 6.05E-05 | 7.03E-05 |
| Total Ion Pump Speed S [L/sec] | 8880 | 8880 |
| Average Pressure P [Torr] | 6.81E-09 | 7.92E-09 |

$$\text{Gas Load } Q \approx EI\eta$$

$$\text{Pressure } P = Q/S$$

Beam Instabilities

PEP-II — DSP based bunch by bunch feedback system

Modular — 15-20 modules to control 1658 bunches

We need 2-3 modules to control 225 bunches

System will also be used at ALS

Magnets

Some X-Ray Ring quads (QC) near saturation at 2.5 GeV

16 new ones needed

Injection

• Present injector can fill x-ray at 1 mA/cycle

• 1.2 injection cycles / second

$$\frac{2400 \text{ mA}}{1 \text{ mA/cycle}} \frac{2 \text{ cycles / second}}{60 \text{ seconds / minutes}} = 48 \text{ minutes}$$

• **TOO LONG!**

• 750 MeV injection implies

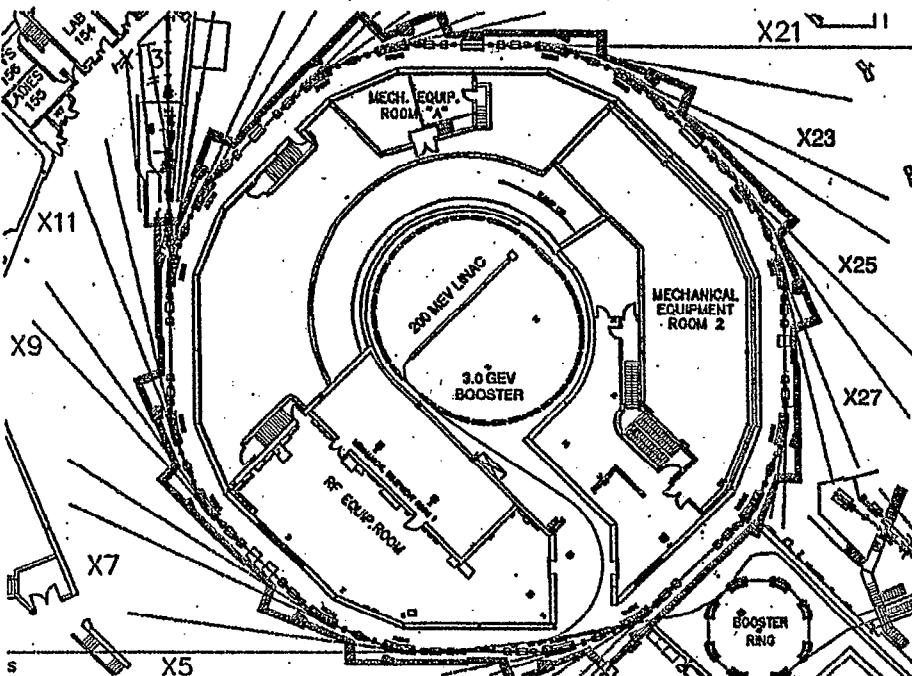
• Large temperature swings in chambers and optics

• Possible beam instabilities at injection energy

HIGH ENERGY BOOSTER SYNCHROTRON

HIGH ENERGY BOOSTER PARAMETERS

| | |
|----------------------------------|----------|
| Current [mA] | 10.00 |
| Repetition Rate [Hz] | 10.00 |
| Acceleration Time [sec] | 0.10 |
| Injection Energy [MeV] | 200.00 |
| Extraction Energy [GeV] | 3.00 |
| Acceleration [KeV/Turn] | 10.59 |
| Revolution Frequency [MHz] | 5.29 |
| Circumference [m] | 56.69 |
| Rf Frequency [MHz] | 475.92 |
| Rf Harmonic | 90.00 |
| Bunches Filled | 75.00 |
| Electrons/Bunch | 1.58E+08 |
| Bend Radius [m] | 6.80 |
| Dipole Magnetic Field [T] | 1.47 |
| Energy Loss/Turn [MeV] | 1.05 |
| Rf Peak Voltage [MV] | 2.00 |
| Overvoltage | 1.88 |
| Synchronous Phase [Deg.] | 32.17 |
| | |
| Number Of Cavities | 2 |
| Gap Voltage/Cavity [MV] | 1.00 |
| Wall Loss/Cavity [KW] | 143 |
| Synchrotron Radiation Power [KW] | 10.5 |
| Total Power Loss [KW] | 296 |
| Number Of Klystrons | 1 |



“B-Factory Upgrade, Science”

Lonny Berman

WORKSHOP ON NSLS UPGRADES

October 23, 2000

B-Factory Upgrade, Science
Lonny Berman

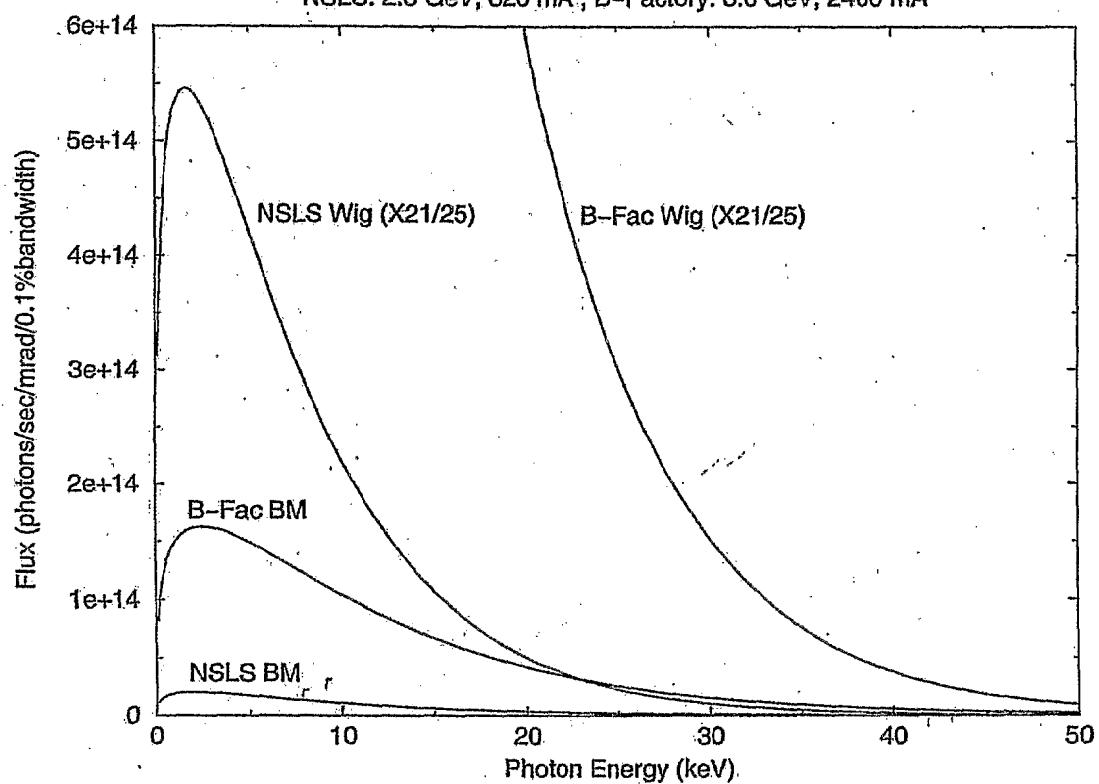
Brookhaven Science Associates
U.S. Department of Energy

1



Flux Comparison of NSLS and B-Factory Sources

NSLS: 2.8 GeV, 320 mA; B-Factory: 3.0 GeV, 2400 mA



B-Factory bending magnet sources are within a factor of 2 of existing X21/25 wiggler sources in hard x-ray range, and 51 out of the 60 x-ray stations presently in operation are bending magnet stations

Optics Demagnification
(by design, not necessarily in practice)

Measured Intensity in Focused Beam

Keeping the same emittance conditions, the B-Factory upgrade
will make the bending magnet focused beam intensities
comparable to what is now obtainable at X25

| Beam Line | Capability | Wavelength Range (Å) | Flux* | Detector |
|-----------|------------|----------------------|-------|----------|
| | | | | |

| | | | | | | |
|------|------|-----------|-----------|----------------------|---|-----|
| NSLS | X4A | MAD | 4-3.1 | 2×10^{10} | ADSC Q4 CCD | 3:1 |
| | X8C | MAD | 0.6-6 | 10^{10} | ADSC Q4 CCD | 1:1 |
| | X9B | MAD | 0.6-3.0 | 1.3×10^{10} | ADSC Q4 CCD <i>mar345</i> Image Plate | 4:1 |
| | X12B | MAD | 0.92-1.61 | 0.6×10^{10} | ADSC Q4 CCD | 1:1 |
| | X12C | MAD | 1-1.6 | 0.5×10^{10} | B1 or B4 CCD | 1:1 |
| | X25 | MAD, Laue | 0.4-4.0 | 1.8×10^{11} | Brandeis B4 CCD | 1:1 |
| | X26C | MAD, Laue | 0.8-3.1 | 0.2×10^{10} | ADSC Q4 CCD Fuji Image Plate | 1:1 |

*measured in 1997 under "old" emittance:

2.584 GeV machine energy

300 mA machine current

12.4 keV photon energy (1Å wavelength)

200 µm crystallography collimator

Si (111) monochromator

horizontal collection of optics:

1 mrad collected on X25

2 mrad collected on dipole lines

Beam Line X21 Scientific Capabilities

High Energy Resolution Inelastic X-Ray Scattering:

- Raman Scattering
- Compton Scattering
- Electronic Excitation Spectroscopy
- Resonant Scattering

Beam Line X25 Scientific Capabilities

High Q Resolution Elastic X-Ray Scattering:

- Surface and Interface Scattering and Reflectivity
- Magnetic Scattering (Resonant and Non-Resonant)
- Speckle and X-Ray Photon Correlation Spectroscopy
- Emission Spectroscopy
- Resonant Nuclear Scattering
- Macromolecular Crystallography
- Small Angle Scattering
- Diffuse Scattering
- X-Ray Standing Waves
- X-Ray Optics

Physics example: liquid $\text{Bi}_{22}\text{In}_{78}$ surface
anomalous reflectivity (X25)

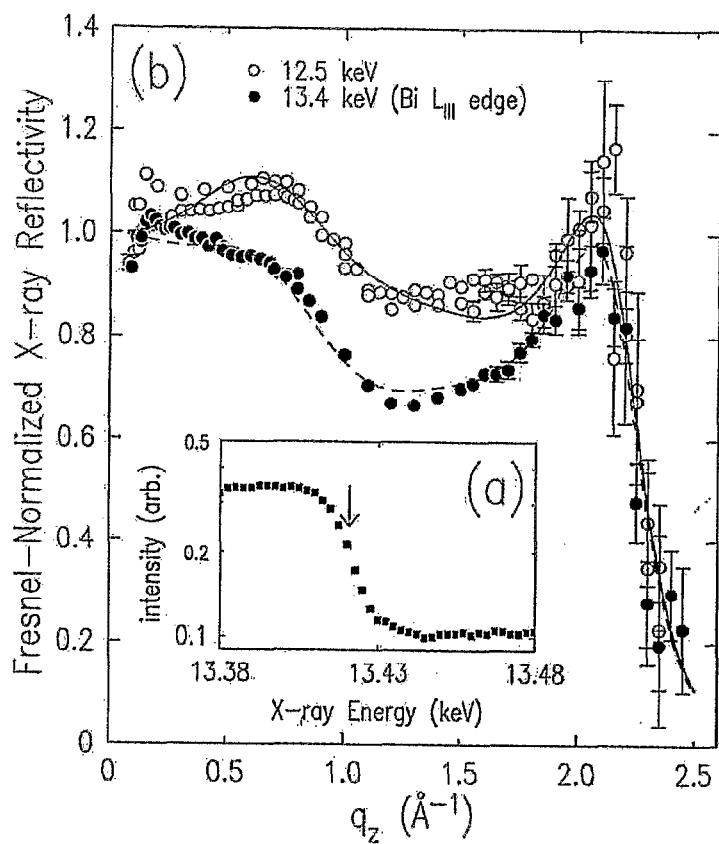
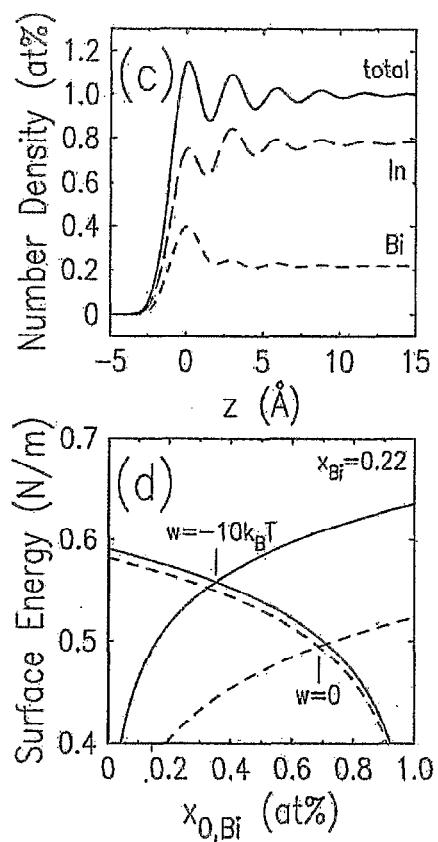


Fig. 1 DiMasi et al PRL submitted)
(BNL, Harvard, Bar-Ilan)

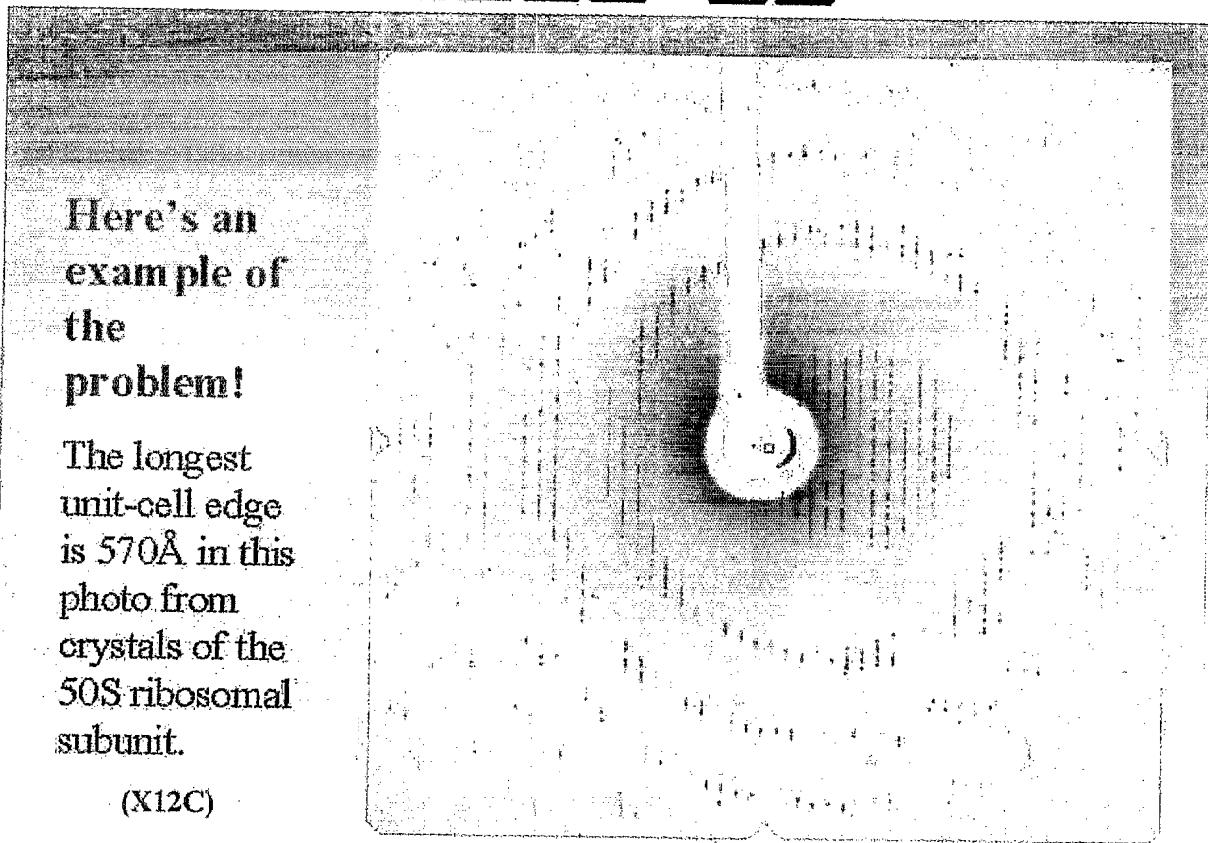


*these sort of profiles, absent of anomalous effects, can be measured
on existing bending magnet lines

*to exploit anomalous scattering in order to quantify the
composition of one component vs the other requires access to X25

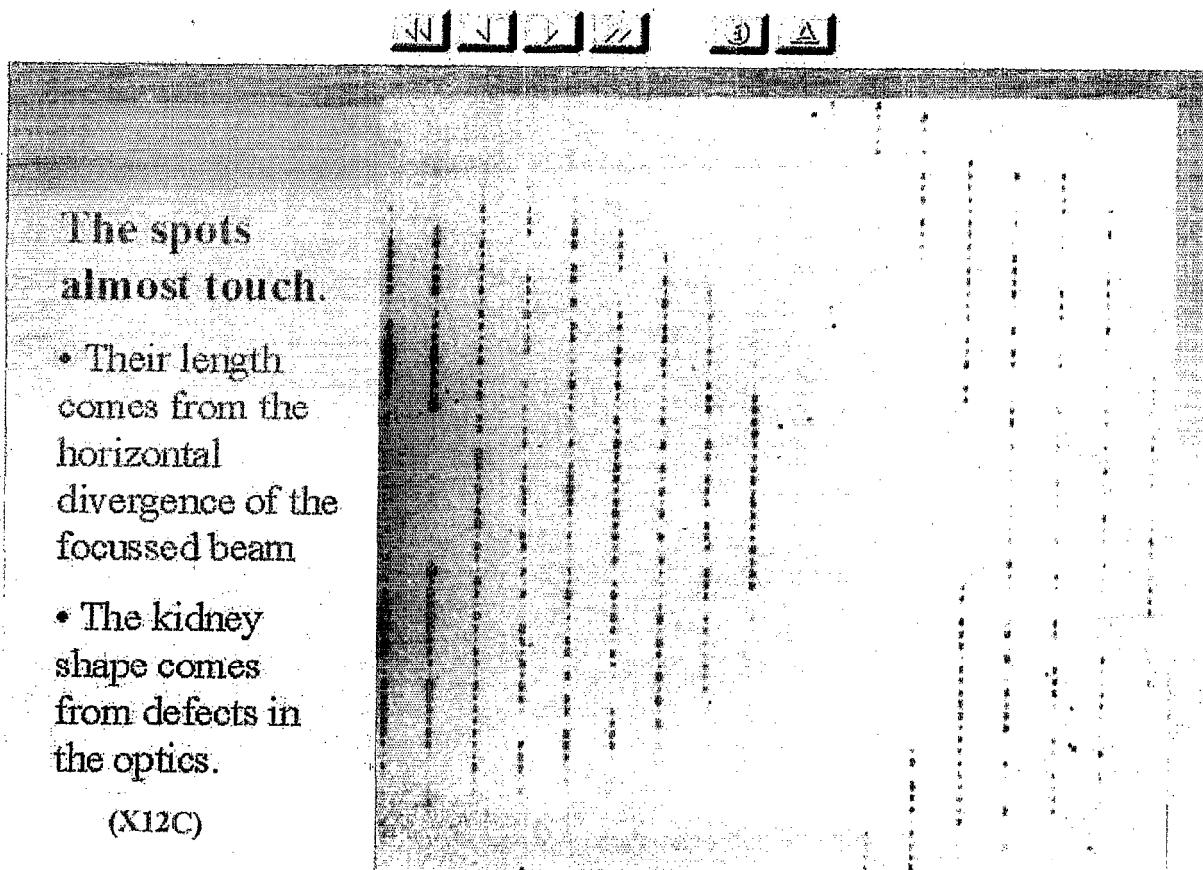
Biology example: ribosome subunit crystallography

Ban et al.
(Yale, BNL)



Rotation diffraction pattern recorded from a single crystal on a CCD area detector (beamline X12C)

Magnified region of diffraction pattern



The spots
almost touch.

- Their length comes from the horizontal divergence of the focussed beam
- The kidney shape comes from defects in the optics.

(X12C)

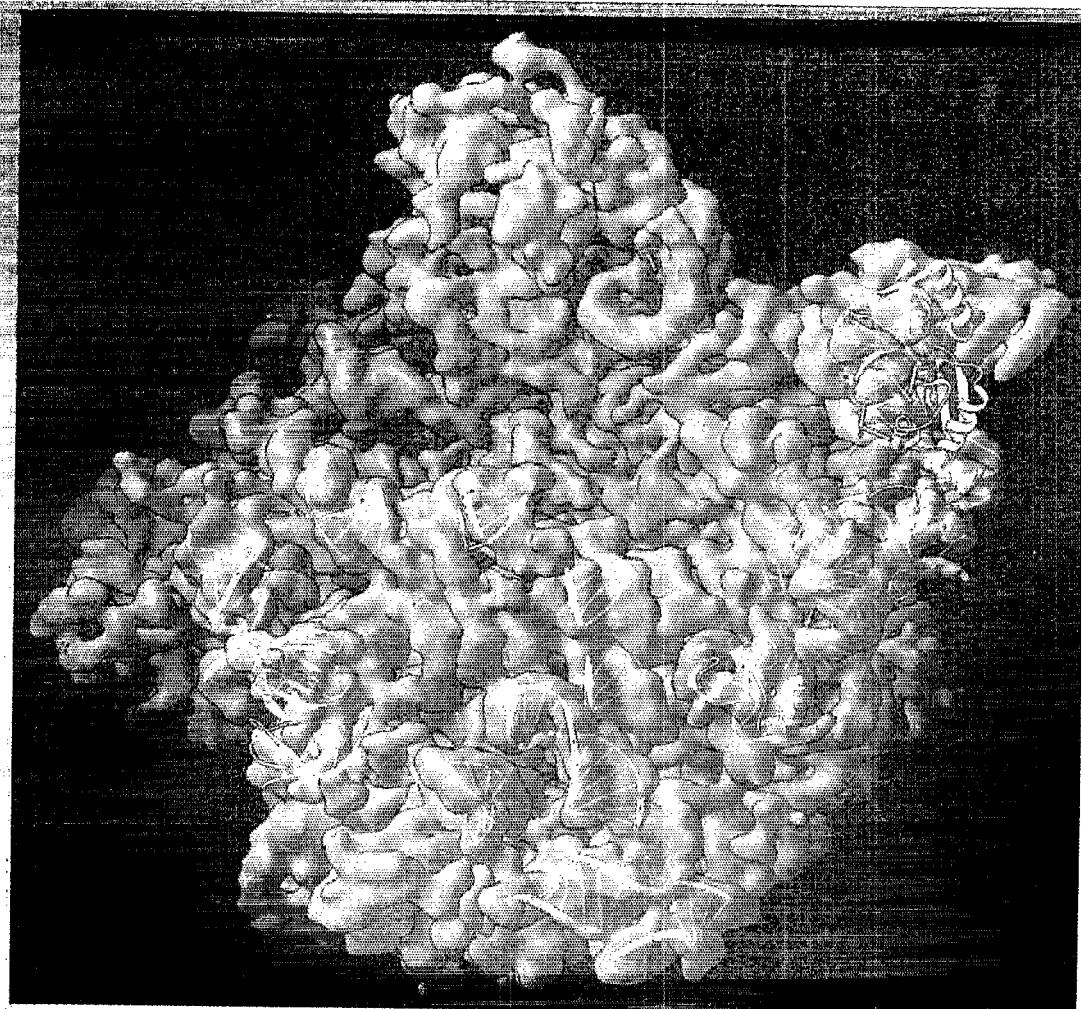
Bax et al. Cell 1998

Brookhaven Biolog

Generally need:

- (1) good collimation to separate spots from large unit structures
- (2) small beam focus because macromolecular crystals are tiny
- (3) decent monochromatization in order to exploit anomalous diffraction (MAD)
- (4) high incident flux because scattering gets weaker at higher momentum transfer
- (5) ergo; high brightness!

5 Å Resolution



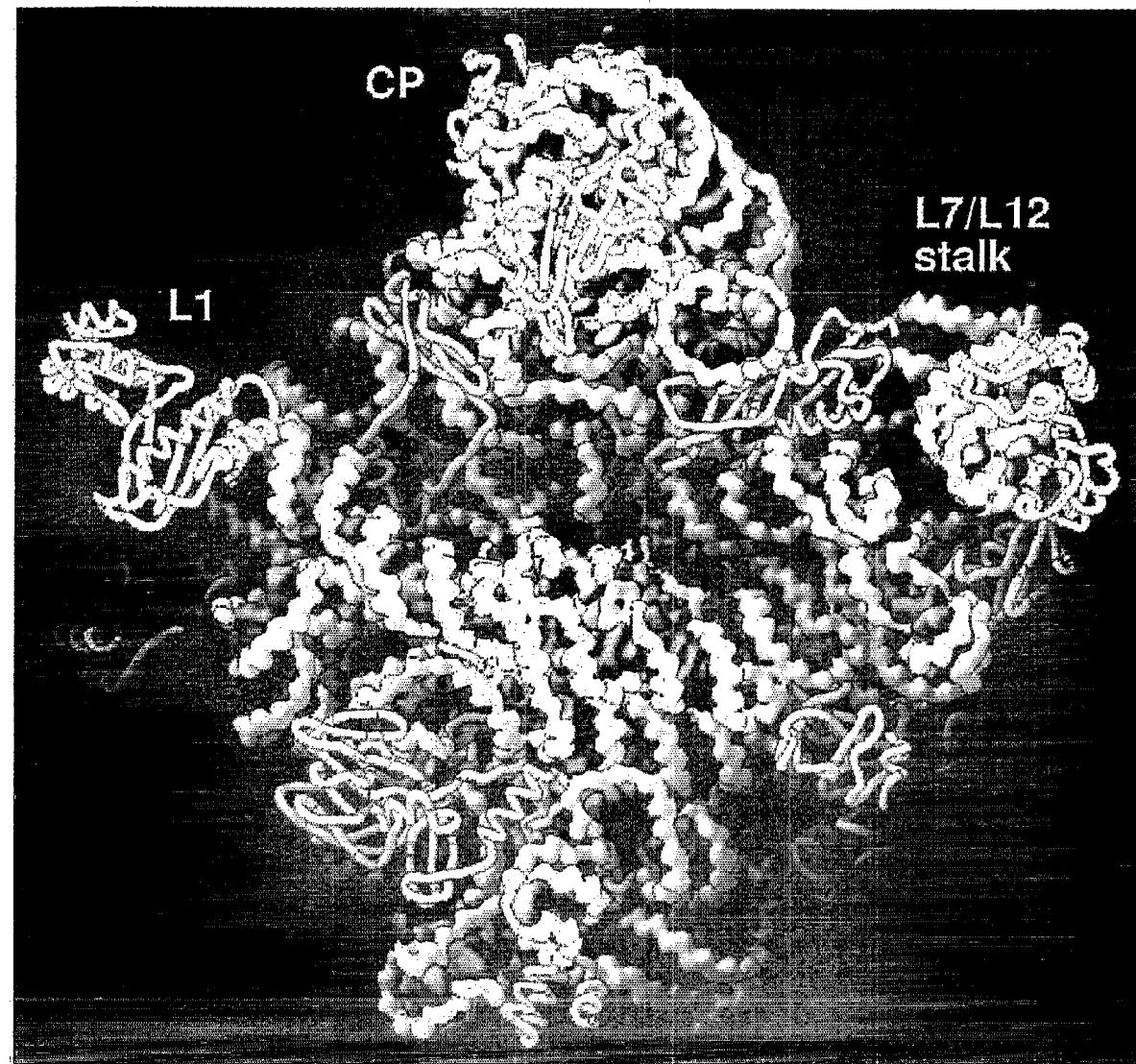
Moore and
Steitz's
groups used
only NSLS
dipole
beamlines to
produce this
model of the
50S subunit

Ban, N., et al. (1998) "A 9Å Resolution X-Ray Crystallographic Map of the Large Ribosomal Subunit." Cell 29, 1105-1115.

Ban, N., et al (1999) "The Large Ribosomal Subunit at 5Å Resolution: Identification of Protein and RNA Structures." Nature 400:841-847.

Brookhaven Biology (X12B, X12C)

50S ribosome subunit, 2.4 Å resolution (X25,APS)

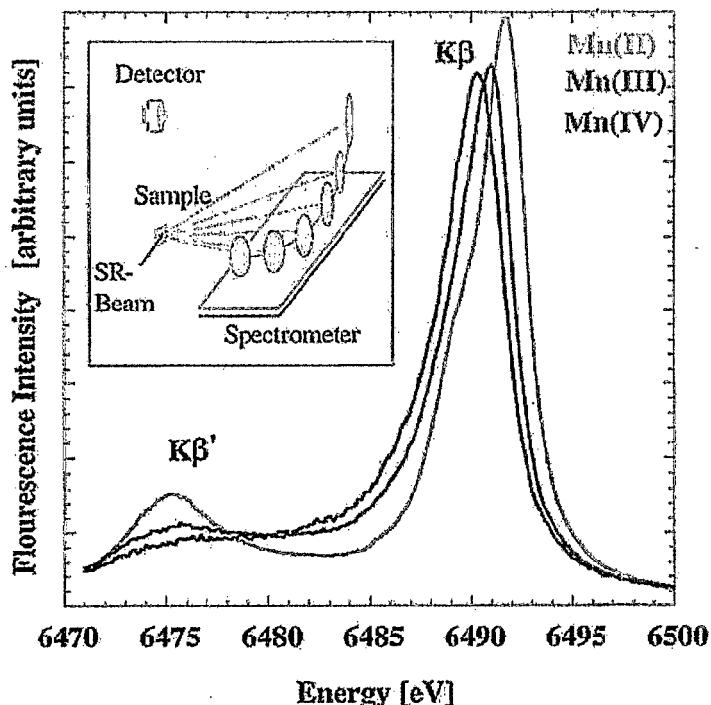


Ban et al,
Science
289, 905-920
(2000)

* this is even a simplification of the true observed image

* to see this level of detail at the atomic level requires access to X25

Chemistry Example: High resolution fluorescence emission spectroscopy
Bergman et al. (LBL, Cal.-Davis)



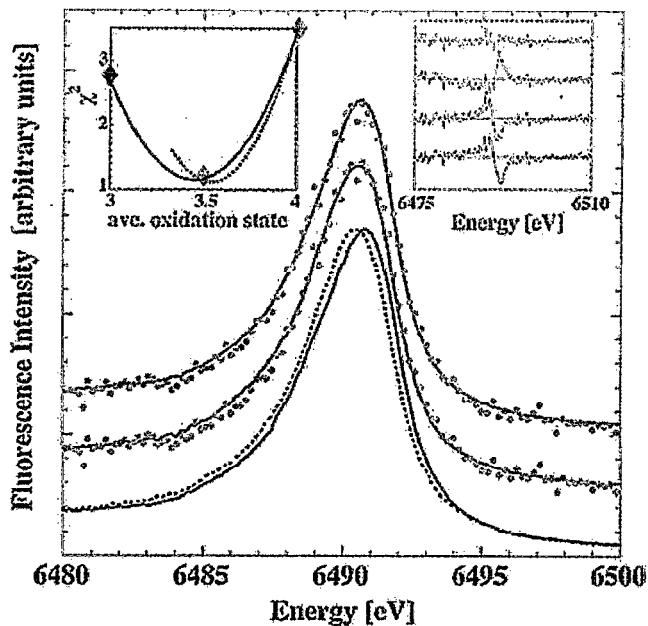
Mn K β emission from different compounds (X25)

Bergman et al.
J.Phys. Chem. B
102, 8350-8352
(1998)

(original synchrotron-based measurement from X25
reported in Hämäläinen et al., Phys. Rev. B
46, 14274-14277 (1992))

Figure 1 K β emission spectra of Mn(II) in MnF₂, Mn(III) in Mn₂O₃, and Mn(IV) in Mn₄O₆(bpea)₄. The spectra are normalized to equal integrated intensities. The same normalization was used to determine the ratio of different models to fit the PSII data. The inset shows the schematic experimental setup.

Mn oxidation states in photosystem II (X25)



Bergmann et al.,
J. Phys. Chem B
102, 8350-8352
(1998)

Figure 2 (Top to bottom) K β emission spectrum of PSII in the dark-adapted S₁ state and best fit using 50% Mn(III) (Mn₂O₃) and 50% Mn(IV) (Mn₄O₆(bpea)₄). K β emission spectrum of PSII in the dark-adapted S₁ state compared with LiMn₂O₄. Spectrum of Mn₁₂O₁₂(O₂CET)₁₆(H₂O)₃ (solid line) compared with LiMn_{1.75}Ni_{0.25}O₄ (dotted line). (Left insert) Values of χ^2 as a function of average oxidation state for two model combinations: models 2 and 3 (solid line) and models 3 and 10 (dotted line). Colored diamonds indicate the average oxidation state and χ^2 -value corresponding to the top three difference spectra in the right insert. (Right insert) Difference spectra (fit minus data) using models 1-3, top to bottom: 50% Mn(III) 50% Mn(IV), 100% Mn(III), 100% Mn(IV), 25% Mn(II) 50% Mn(III) 25% Mn(IV).

^abulk compounds can be measured easily on existing bending magnet lines
with this sort of sophisticated spectrometer.
^bhowever, dilute species (e.g. metalloproteins) require X25

NiK $\beta_{1,3}$ emission in photo-excited Ni-containing metallo-proteins (X25)
Glatzel et al (Cal.-Davis, LBL, Nebraska)

Carbon monoxide dehydrogenase

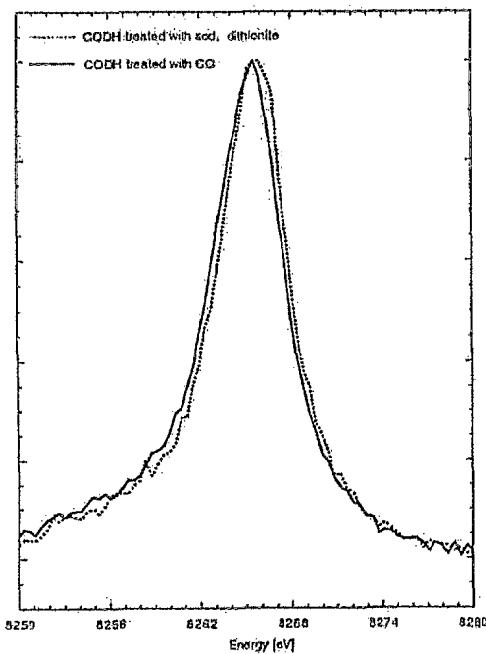


Figure 1. K $\beta_{1,3}$ lines of CODH

Hydrogenase

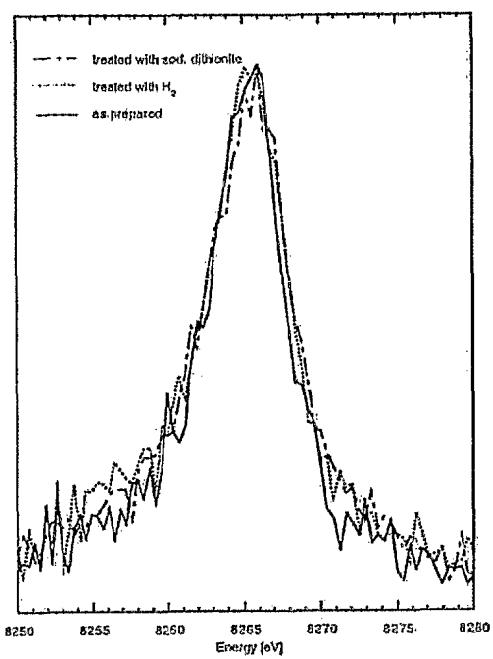


Figure 2. K $\beta_{1,3}$ lines of hydrogenase

* This research was supported by the NIH, grant GM-48145

Table 1: Statistics of X25-Derived Publications
(NSLS in microcosm)

| Fiscal Year | Total Papers | Non-Macro-crystallography | Macro-crystallography | Cell | Nature | Physical Review Letters | Science | Physics | Biology |
|-------------|--------------|---------------------------|-----------------------|------|--------|-------------------------|---------|---------|---------|
| 1991 | 5 | 5 | 0 | 0 | 1 | 0 | 0 | 1 | 0 |
| 1992 | 15 | 14 | 1 | 0 | 0 | 1 | 0 | 1 | 0 |
| 1993 | 16 | 15 | 1 | 0 | 0 | 1 | 0 | 4 | 0 |
| 1994 | 18 | 15 | 3 | 0 | 0 | 3 | 1 | 2 | 1 |
| 1995 | 12 | 10 | 2 | 0 | 4 | 2 | 0 | 4 | 2 |
| 1996 | 15 | 10 | 5 | 2 | 2 | 4 | 0 | 4 | 5 |
| 1997 | 19 | 10 | 9 | 1 | 6 | 4 | 0 | 2 | 6 |
| 1998 | 24 | 13 | 11 | 2 | 3 | 1 | 1 | 1 | 6 |
| 1999 | 25 | 11 | 14 | 5 | 2 | 2 | 2 | 1 | 9 |
| 2000 | 43 | 10 | 36 | 3 | 2 | 1 | 5 | 2 | 10 |
| Total | 133 | 113 | 86 | 23 | 20 | 19 | 9 | 39 | 39 |

↑ ↑
physics structural biology
chemistry
materials science

high-profile
journal
totals

Why such a tremendous jump in macro-crystallography publications in fiscal year 2000? Only sensible explanation seems to be the factor of 2 increase in user support, on behalf of structural biology, made possible by the new NIH/NCRR Research Resource grant for several NSLS biology beam lines (commenced in fiscal year 1999).

**Construction of a
New Storage Ring of
Conventional
Design, Such as
Diamond or the
Swiss Light Source**

“New Storage Ring, Accelerator”

James B. Murphy

3rd Generation X-Ray Rings

J.B. Murphy
NSLS/BNL

NSLS Workshop on
Future Sources
October 23, 2000

Outline

- o What is a 3rd Generation X-Ray Ring?
- o Storage Ring Quality Factors
- o Insertion Device Capacity
- o Emittance/Brightness/Pulse Duration
- o 3rd Gen. Source in the X-Ray Tunnel
- o Costs
- o Concluding Remarks

What is a 3rd Generation X-Ray Ring?

- Same as the 2nd generation but with a larger number of basic cells to reduce ϵ and increase ID capacity
- Challenges: dynamic aperture, stability, lifetime, cost, ...
- New Technologies: SRF, ...

Storage Ring Quality Factors

| | |
|--|--|
| <u>Capacity</u> $N_{ID} \gg 1$ | <u>Emittance</u> $\epsilon_x \propto F(v_x) \frac{E^2}{N_{cell}^3}$ |
| <u>Brightness</u> $B \propto \frac{IL_u}{(\epsilon_x + \lambda/2)(\epsilon_y + \lambda/2)}$ | <u>Cost</u> $\$ < \$_{limit}$ |

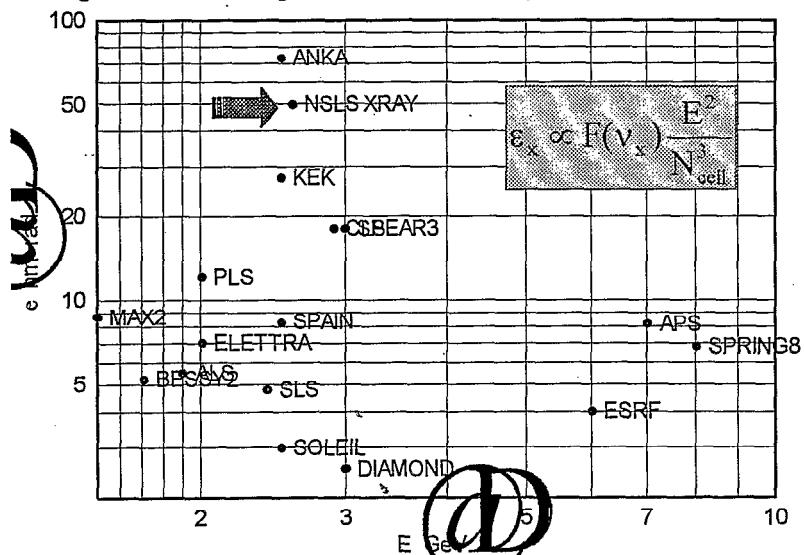
Insertion Device Capacity

| Ring | E (GeV) | C (m) | Straights | |
|-------------|------------|------------|-----------|-----------|
| SLS | 2.4 | 288 | 3L/3M/6S | |
| ANKA | 2.5 | 110 | 4L/4S | |
| SOLEIL | 2.5 | 337 | 4L/12M | |
| NSLS | 2.8 | 170 | 8M | =2 x NSLS |
| CLS | 2.9 | 171 | 12 | |
| BOOMERANG | 3 | 164 | 6L/6S | |
| SPEAR 3 | 3 | 234 | 4L/16S | |
| DIAMOND | 3 | 489 | 6L/18M | =3 x NSLS |

- New rings have 2-3 times ID capacity of the NSLS
- But they're roughly 2-3 times the circumference!

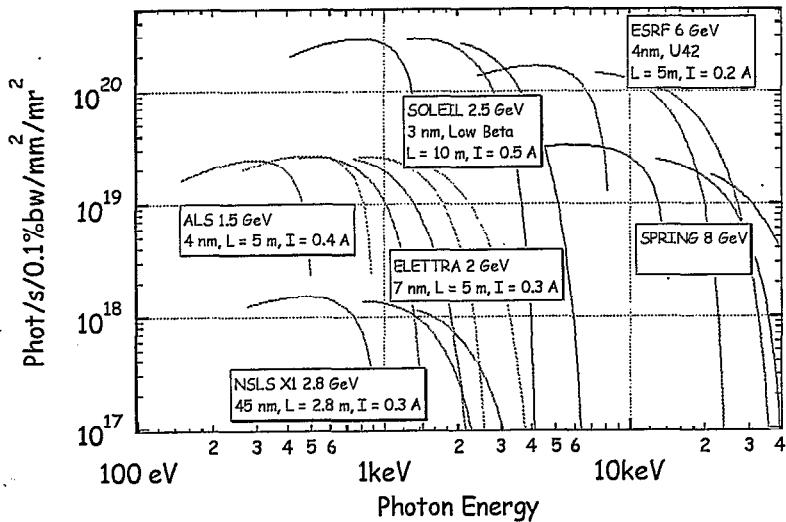
Emittance of X-Ray Rings

3rd generation rings can reduce ϵ by a factor of 15



Undulator Brightness

3rd generation rings can increase brightness by 10²



Electron Bunch Length/Pulse Duration

| Ring | E [GeV] | σ_L [ps] |
|-----------|---------|-----------------|
| ALS | 1.5 | 14 |
| SLS | 2.4 | 13 |
| SOLEIL | 2.5 | 12 |
| NSLS XRAY | 2.8 | 158 |
| DIAMOND | 3 | 10 |
| ESRF | 6 | 16 |

- Low frequency RF at NSLS means $\sigma_L \sim 160$ ps
- 3rd gen sources have $\sigma_L \sim 12$ ps, not 67 fs ala LCLS!

Canadian Light Source in the NSLS X-Ray Ring Tunnel

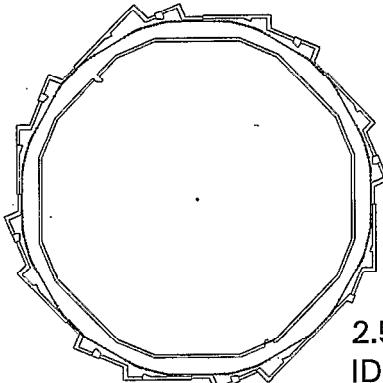


Figure Courtesy of S. Pjerov

- + C ~ 170/171 m
- + E ~ 2.8/2.9 GeV
- + N_s = 8/12
- + ε = 45/18 nm-rad
- β_y = 0.35/4.6 m

2.5x lower emittance & 50% more ID capacity, sans small gap, is possible but the retrofit will be costly & need a 2+ yr shutdown

Notes on Costs

- A ALS Design Book in 1990 M\$ / estimate with 4% escalation for 10 yrs.
- B SLS from L. Rivkin 9/00, with 7.5% tax & no manpower, 4.5 beamlines
- C ANKA from D. Einfeld, 10/00, 9 beamlines, clean room
- D SOLEIL from M.P. Level, 10/00, 1998 cost escalated by 2% to give 2000 cost, 24 beamlines, no VAT
- E CLS Design Book from S. Hulbert 9/00
- F SPEAR 3 from R. Hettel, 9/00, machine w/20% contingency + overhead, beamlines w/burden
- G DIAMOND from M. Poole, 10/00, 2000 cost (\pm 20 %), 24 cells, 7/15 beam lines, inc full staff costs, no VAT. Estimate not yet ratified.
- H APS from J. Galayda

Summary

Key Issues: ID capacity & average brightness

3rd generation sources, while challenging, are mostly an extension of existing technology; however they offer the following enhancements over the NSLS,

- o ID capacity & circumference are 2-3x NSLS
- o Horizontal emittance can be reduced by 15
- o Brightness can be increased by 10²
- o Pulse duration is tens of ps, not tens of fs

Closing Remarks

- o Significant improvements in the quantity & quality of photons are possible with a 3rd generation ring
- o Steady state 100 fs pulses are not possible
- o New ring is preferable to retrofit/shutdown
- o SOLEIL or DIAMOND size offers most gain
- o Cost guestimate ~ 1/4 - 1/3 gigabuck
- o Is there enough bang for the buck?

“New Storage Ring, Science”

Erik Johnson

Scientific Potential from a Third Generation Storage Ring

Advantages of 'Third Generation' SR vs. existing NSLS

Enhanced Brightness

Enhanced Beamline Optics
Performance

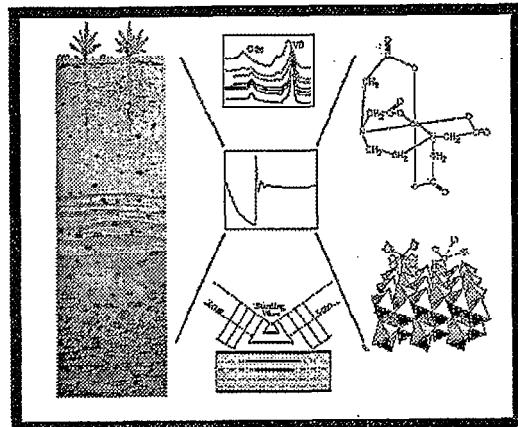
More Available ID's

Enhanced Photon Flux
on Sample

Illustrate with some examples from existing research

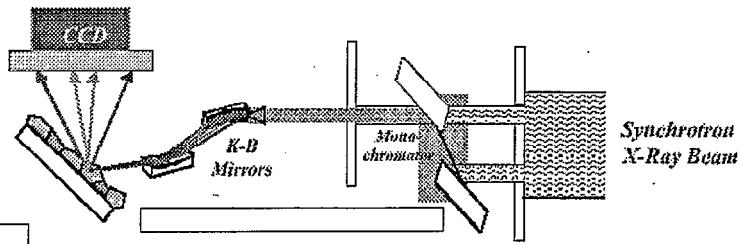
Molecular Environmental Science And Synchrotron Radiation Facilities

1995 DOE Airlie Workshop on MES and updates



- Many Findings and Recommendations with respect to Synchrotron Radiation based Research for MES
- Microprobe Tools have a significant role at spatial resolution
 - 10 μm

X-ray Microprobe



White light or monochromatic beam

Demagnify source (synchrotron) to probe beam

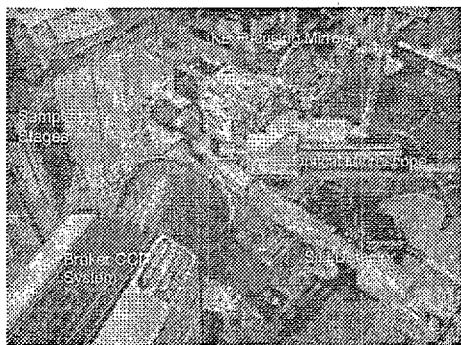
Scan Sample through beam

White light or monochromatic illumination

Diffraction, Fluorescence, or Transmission Detection

Selected area spectroscopy possible

X-ray Microprobe at X26A



University of Chicago – Consortium for Advanced Radiation Sources

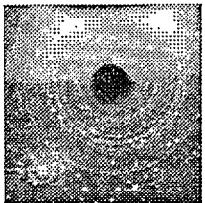
BNL - Environmental Sciences Department

University of Georgia - Savannah River Ecology Laboratory

Spot Size 10 – 200 μm^2 typical

Flux 7×10^{10} White beam

7×10^7 Monochromatic (10^{-4})

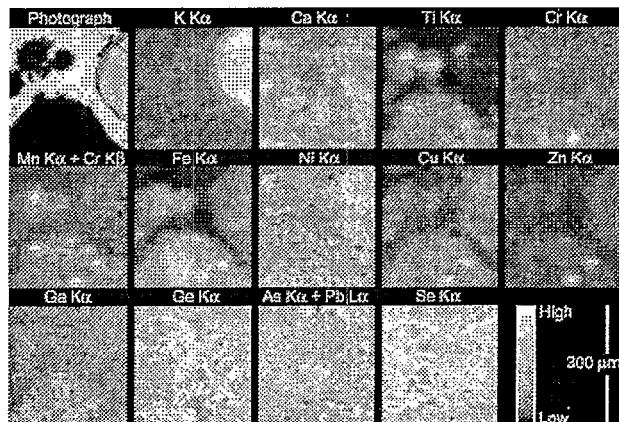


10 μm dia olivine aggregate

1999 NSLS Activity Report;
26 Contributions
16 Publications for FY 1999

New Combined Micro-diffraction and Micro-XAFS Studies at the X26A Beamline, 1999 NSLS Activity Report, A. Lanzilli, S. Sutton, J. Parise, M Vaughn

**Microscale Heterogeneities in Brazilian Oxisols, J.J. Marques, D.G. Schulze, N. Curi,
X26A 1999 NSLS Activity Report**



**13 keV
Monochromatic beam**

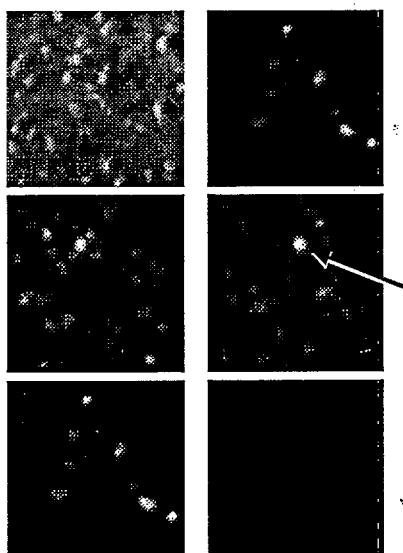
**12 x 17 μm
spot 10 μm step size**

**Detection Limits
~ 1-5 ppm**

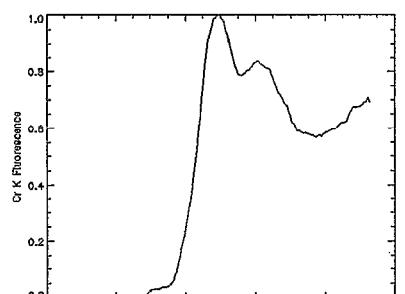
Thin section x-ray fluorescence microprobe

**X-ray Microprobe Results – Soil 3P
W. Bleam, M. Szulczeński; Wisconsin
May 1998, Prepared by Steve Sutton U. Chicago**

GSECARS, APS Sector 13
<http://cars9.uchicago.edu/gsecars/>



**6 keV Monochromatic beam
4 x 4 μm spot 10 μm step size
500x500 μm scan, 2s per step
Detection Limits ~ 100 ppb**



**Spot Size ~ 25 μm^2 typical
Flux 1×10^{13} Monochromatic (2×10^{-4})**

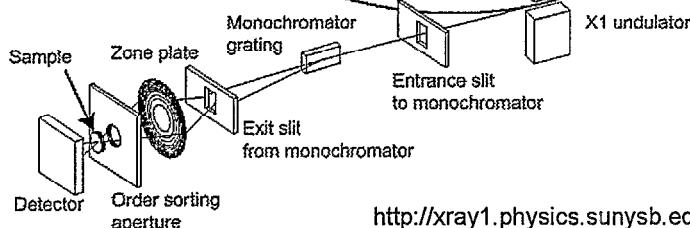
Zone Plate Microscopy

- ❑ Soft X-rays Water Window
- ❑ Specimens in air or 'wet'
- ❑ Limit to probe size

ZP outer zone width

Coherence of source

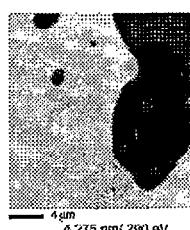
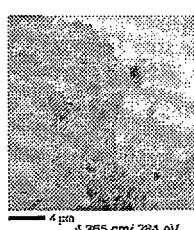
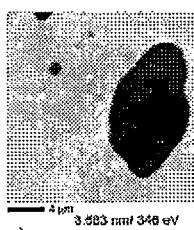
- ❑ Beams ~ 30 nm



<http://xray1.physics.sunysb.edu/>



Solid stabilized water/oil emulsion (X1A ~ 1998)



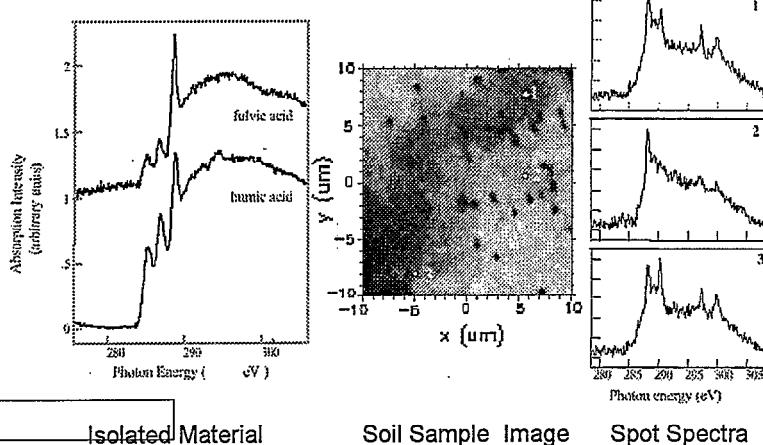
Adjust energy of light
to adjust contrast

Clay + Ca/Al double
hydroxide (LDH) +
Oil + Water

Determine distribution
of components to
understand structure
of heterocoagulates

Humic substances in pine ultisol aggregates in water (BL7.0 ALS ~ 1999)

C-NEXAFS



S. Myneni, LBNL

Comparison of STXM images

Advantages of 'Third Generation' SR vs. existing NSLS

Enhanced Brightness

ALS U5 ~ 10-20 x X1A)

Spatial Resolution comparable (30 to 50 nm)

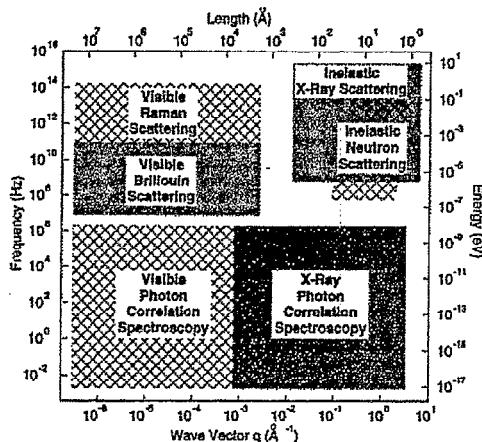
Can use 'extra' photons in Monochromator

Improve spectral resolution or

Reduce dwell time per pixel

In practice 'advantages' are very problem specific and generally no more than ~x10 in some parameter

Photon Correlation Spectroscopy (Speckle)

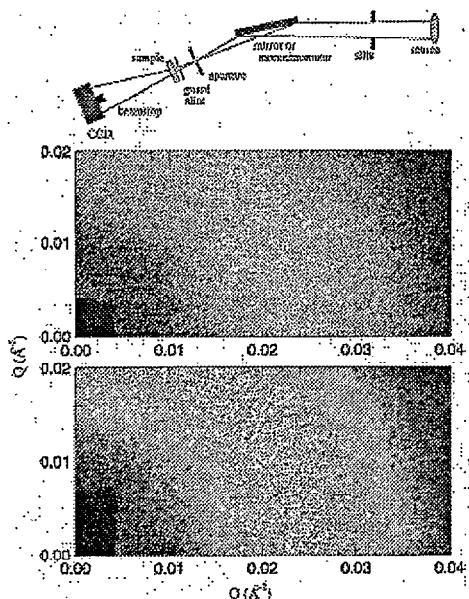


Probes low frequency dynamics of a material by analyzing the temporal correlations among photons scattered by material

Requires transverse and longitudinal coherence

Steve Dierker, 1995 NSLS Newsletter

An example from ESRF (ID10A)



Schematic view of the Troika beamline for using coherent x-rays (a), plus small-angle speckle patterns obtained using monochromatic (b) and "pink" (c) beam conditions. The diffraction patterns from the porous glass Vycor are shown in the wavevector range from 0 to 0.04\AA^{-1} horizontally and 0 to 0.02\AA^{-1} vertically.

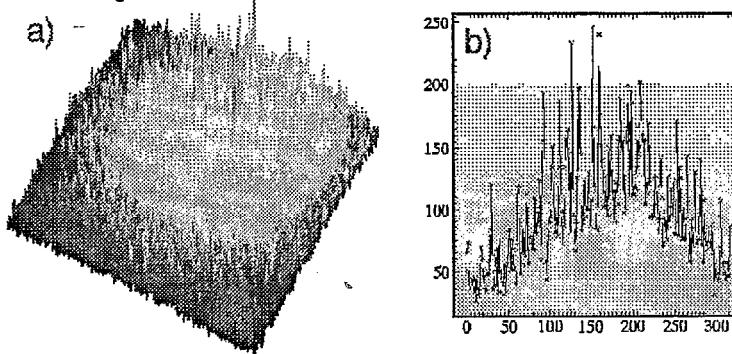
Small angle scattering from ferrofluid in zero and applied magnetic field



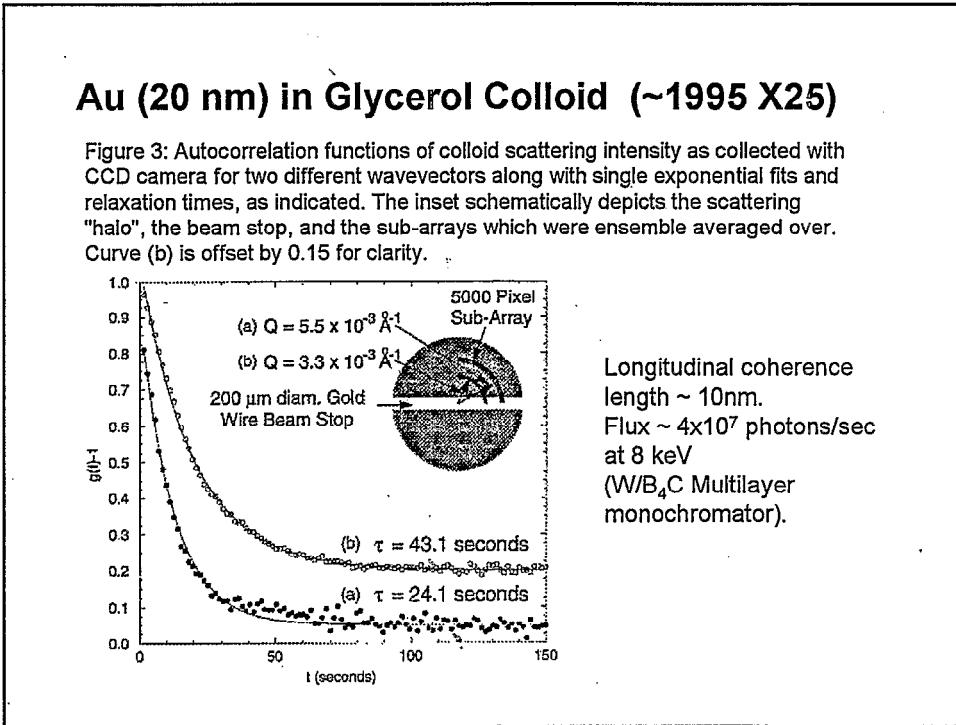
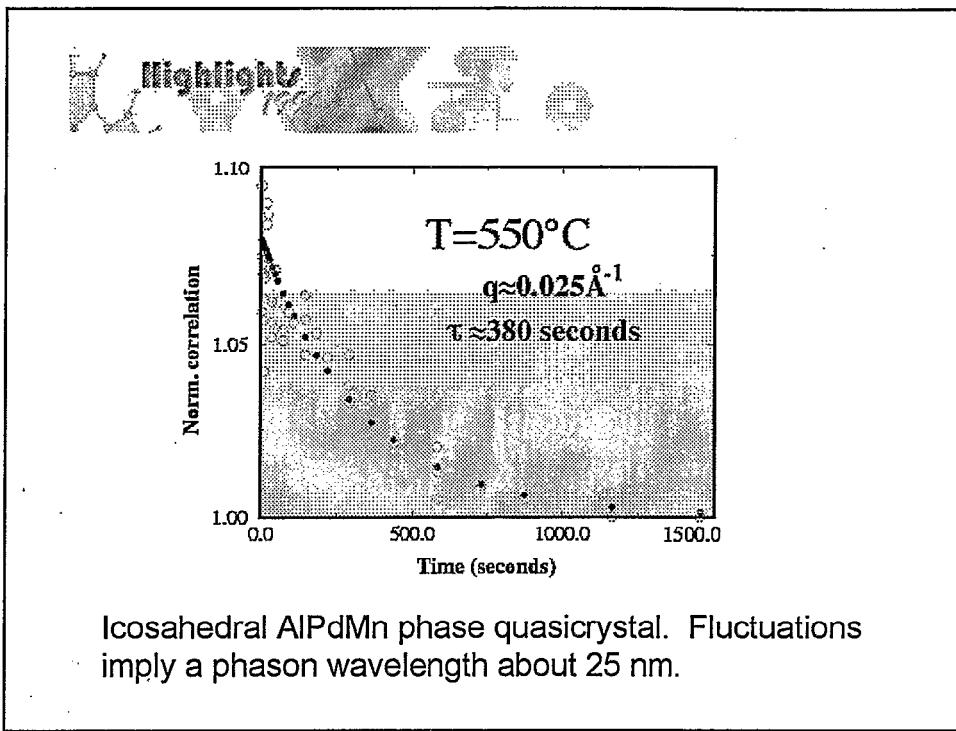
<http://www.esrf.fr/info/science/highlights/97-98/PF116.htm>

Coherent X-ray Diffraction and Phasons Fluctuations in Quasicrystals (ESRF ID20)

Fig. 56: (a) 2-D image of the speckle pattern taken in the diffuse tails of a Bragg reflection (b) slice through Figure 56a. Intensity fluctuations are much larger than the counting statistics.



Beam coherence (~40%) achieved with 10 μm pinhole 1.8 m from sample 7×10^8 photons/sec at 7.6 keV (Si 111 monochromator).



X-ray Photon Correlation Spectroscopy . . .

Advantages of 'Third Generation' SR vs. existing NSLS

Enhanced Brightness

Coherent Flux enhanced $\sim x10^2$ or $x 10^3$
for comparable longitudinal coherence length

Systems thus far 'special cases'

Extending the generality of this technique requires a more powerful coherent source (ala LCLS) and in fact is one of the elements of the proposed 'First Experiments'

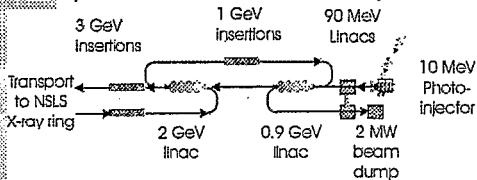
Construction of Linac-Based Sources

“Energy-Recovery Linac Sources”

Ilan Ben-Zvi

Layout for an Energy Recovering Linac for the NSLS

- Limit energy ratio of the beams in any one linac section (Dave Douglas).
- Inject at high energy.
- 10 MeV source has no energy recovery (RF power loss: 2 MW plus cavity loss)
- Beam dump: 2 MW minus SR power. Below neutron generation threshold.
- 90 MeV pre-accelerator – possibly separate function unit for recovery.



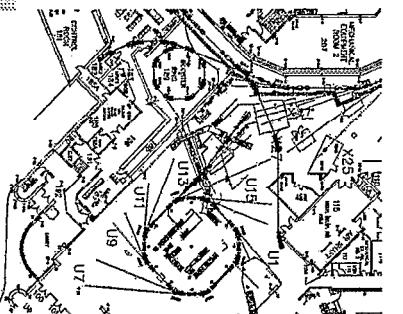
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BNL, October 23, 2000



Integration into the NSLS

- Turn off one magnet – (need new magnet chamber)
- Connecting beam line have minimal interference

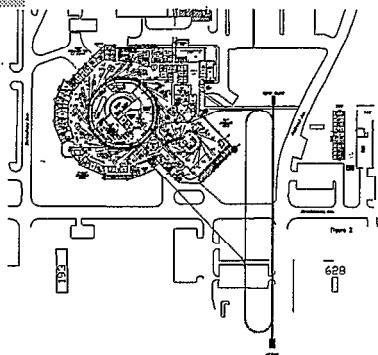


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A possible layout (for scaling purposes only)



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Linac Beam Parameters

| Parameter | Units | Value |
|---|-------------------------------|----------------------|
| Energy, single pass | GeV | 3 |
| Average current | Amperes | 0.2 |
| Bunch repetition frequency | GHz | 0.433 / 1.3 |
| Bunch charge | nC | 0.45 / 0.15 |
| rms emittance: Normalized - Geometrical - | μm \AA | 1 / 0.5 1.7 / 0.8 |

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Emittance – How Small?

- The numbers used are based on ATF results and known scaling.
- Possible improvement by about a factor of 2-3, by optimizing parameters for a lower charge and shaping the laser profile.
- Thermal emittance $\varepsilon_{th} \sim 0.25R_c$, where ε_{th} is in μm , R_c in mm. This may become a limit below 0.2 μm .

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Bunch-length: How short?

This depends on:

- How much energy spread?
 - JLAB FEL measured 0.175 MeV-ps, that is 0.06% \times 100fs at 3 GeV.
- In which beam lines?
 - With the NSLS normal momentum compaction $\alpha=5.6\times 10^{-3}$, at an energy spread of 0.06% the bunch will elongate by 1 ps after half a turn. One may consider reducing α .
 - The temporal 'beam waist' may be placed at any point along the ring.
 - Insertion devices may be placed before the X-ray ring for sub 100 fs operation, with ~ps bunch length over most of the ring.
- With what emittance? Theory not ready for ultra short bunches at 10 fs FWHM. Low charge helps.

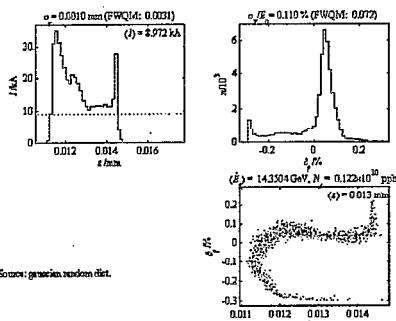
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LCLS at 15 GeV Two Bunch Compressors. Short Bunch Task-Force:

- Nominal: 1 nC, $\epsilon_n \sim 1.5 \mu\text{m}$, 255 fs FWHM
 $\Delta p/p \sim 0.06\%$ FWHM.
- 0.2 nC, 10 fs FWHM $\Delta p/p \sim 0.07\%$ FWHM
(modified settings). Emittance not evaluated.



Source: generation random dist.

ket_id: LCIS-38 with new_gen_dist,
17-APR-2010 13:08:29; 1/27000000

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Extreme flexibility on a fast time scale.

- The basic pulse format is a repetition rate of 0.433 or 1.3 GHz, bunch charge of 0.45 or 0.15 nC (for 200 mA).
- Laser opto-electronic control of charge.
- At a given current, larger bunch charge with a lower rep rate (emittance increases with bunch charge).
- Mixed bunch families:
 - Charge / emittance
 - Bunch length
- Extract secondary beam(s).
- Change emittance ratio ϵ_x/ϵ_y (on a slower time scale).

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The Superconducting Electron Linac

- Extremely well known (JLAB, DESY, industry). Assume TESLA cavities:
- $R/Q = 1036 \Omega$, $L = 1.038\text{m}$
- Take conservatively $Q_0 = 1.5 \times 10^{10}$ at 2K, 20MV/m, 150 cavities
- Refrigeration power 26 W/structure
- 4kW refrigeration (~2.5 MW plug power)
CEBAF is 5 kW (16M\$), upgrade to 10 kW
- HOM power: (Merminga et. al., LINAC2000) At eRHIC, due to the 20 ps pulse length, this is not a problem.

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TESLA Accelerator Structure

- Highly optimized, well characterized
- A number of manufacturers
- Improvements still being made

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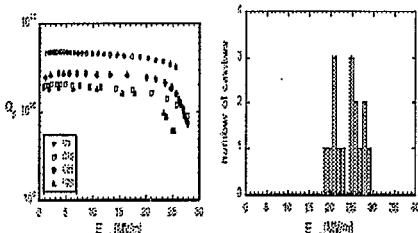
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Performance of TESLA Cavities

- Residual resistance $3 \text{ n}\Omega$, equiv. to a Q of 10^{11} .
 - Optimization was towards high gradient, not Q. Expect improvement in Q, (Kneisel – furnace baking doubles Q_{BCS})
 - Q vs. E: Best cavity, 4 manufacturers, at 2K. Note high Q at 20 MV/m:



III. B. (iii) consequences of the last cell division of each of the last two generations. (iv) The fraction of maximum product for each subset of class I, starting a quality from $Q = 5\%$?

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The Electron Source: Photocathode Material

- K₂CsSb well developed at LANL, Boeing and other places. QE ~5% at green light, lifetime well over 10 hours at vacuum of 8×10^{-10} .
 - Cesium telluride (Cs₂Te) cathodes are more robust. QE ~5% at UV. Survive weeks in vacuum of 10^{-9}
 - P(laser at IR)=I*hv/(Conv*QE)
 - For green: hv=2.5 eV, Conv~0.3 P~30 W, current technology.
 - For UV: hv=5 eV, Conv~0.06 P~300 W, near future / multiple lasers.

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The Electron Source. One Possibility: The Boeing Gun

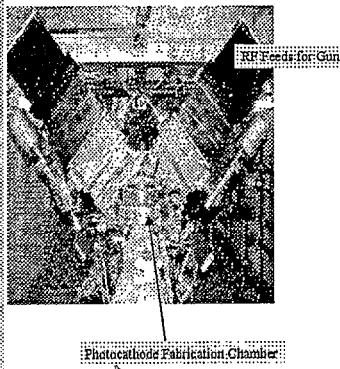
- Operated 433 MHz photoinjector
 - Tested at 25% duty factor (klystron limited). CW possible.
 - Typical 135 mA average current during macropulse, using 13 W Nd:YLF laser.
 - 5 MeV injector (2 MeV out of gun, 3 MeV in two additional cells), 4 MW total power at peak.
 - 26 MV/m on cathode
 - K₂CsSb cathode QE 5% to 12%
 - 10 hour lifetime at 10⁻⁹ torr (RF on)
 - 4 μm emittance at 1 nC (severe coil misalignment, Gaussian laser)

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The Boeing 433 MHz RF Photocathode Gun

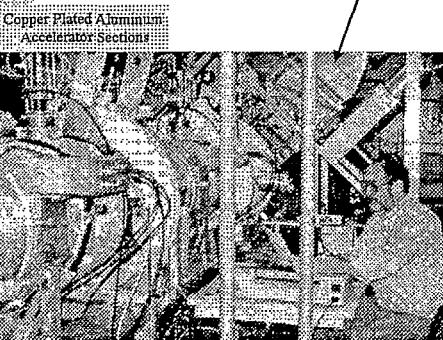


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The Boeing 433 MHz, CW Accelerator Sections



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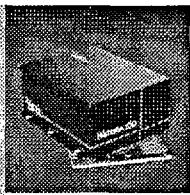
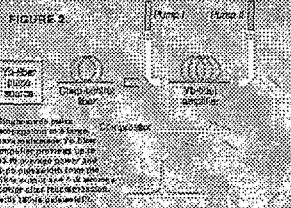
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A Possible Photocathode Laser

Recent Development at IMRA America, Inc.

- Seed laser: 300 mW, 1055 nm, 2-ps, 50 MHz.
- Power amplifier: 4.3-m of Yb-doped fiber.
- Pump: Two fiber-bundle-coupled laser-diode sources at 976 nm. Slope efficiency 50%.
- Maximum amplified power 13 W (diffraction-limited) pulse width 5 ps (pulse energy 0.26 μ J), Expect >100W in the future.
- Ultra-stable, compact, rapidly-evolving.

13W development (larger fiber) Off the shelf 1W unit



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Beam Breakup in the Combined Function Linac

- Multipass Multibunch Instability (100 mA) (Lia Merminga).
- With B-factory style feedback expect large improvement (Geoff Krafft, John Fox).

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Beam Stability

■ Position

- Expected beam size 10 μm .
- Linear collider – stability better than linac beam size in a low rep rate pulsed machine.
- Control improves with bunch repetition rate. Great advantage to GHz class bunch rate.
- Ultimate limit ground motion. 10-100 nm ground stability established in accelerator sites.

■ Current

- Diode pumped lasers <1% stability

■ Energy

- CEBAF energy stability 2.5×10^{-5}

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Accelerator Physics - What Next?

■ Challenges: Establish new technology at BNL, increase current by factor of ~40.

- Theory:

- Lattice design
- Low emittance conditions in gun
- Compression, Emittance growth
- Instabilities
- Feed-back

- Experiment:

- RF gun and laser:
 - Current, emittance, amplitude stability
- Superconducting linac section:
 - Feed-back, BBU, stability, energy recovery

- Design X-ray insertions and beam lines

- Engage NSLS users
- Establish desired parameters

■ CDR

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“Free-Electron Lasers”

Li-Hua Yu

High Gain Harmonic Generation Free-Electron Lasers

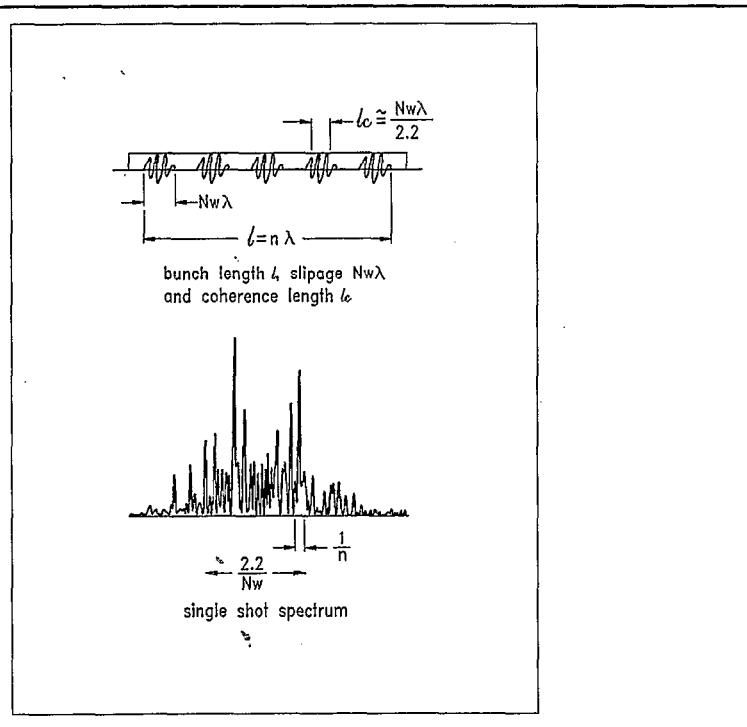
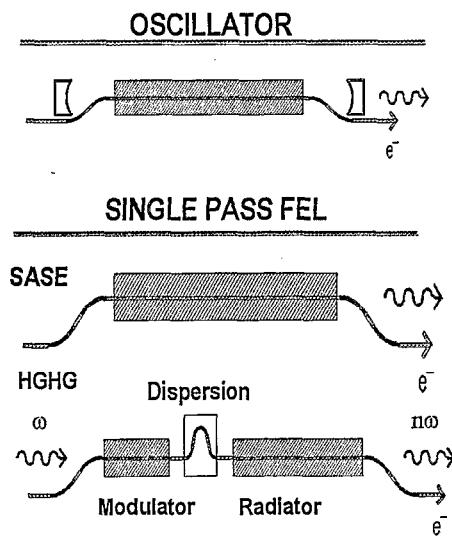
Li Hua Yu

NSLS Upgrade Workshop, Oct. 2000

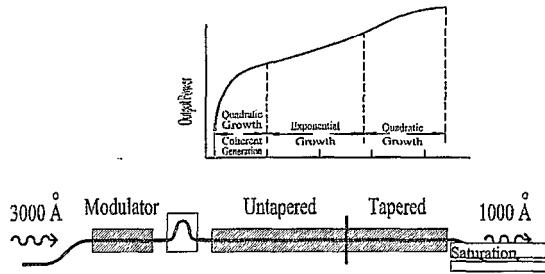
Outline

- Different approaches to x-ray FEL
- HGHG approach to achieve full coherence
- Recent proof of principle experiment of HGHG
- How to achieve hard x-ray? Cascading HGHG

FEL CONFIGURATIONS

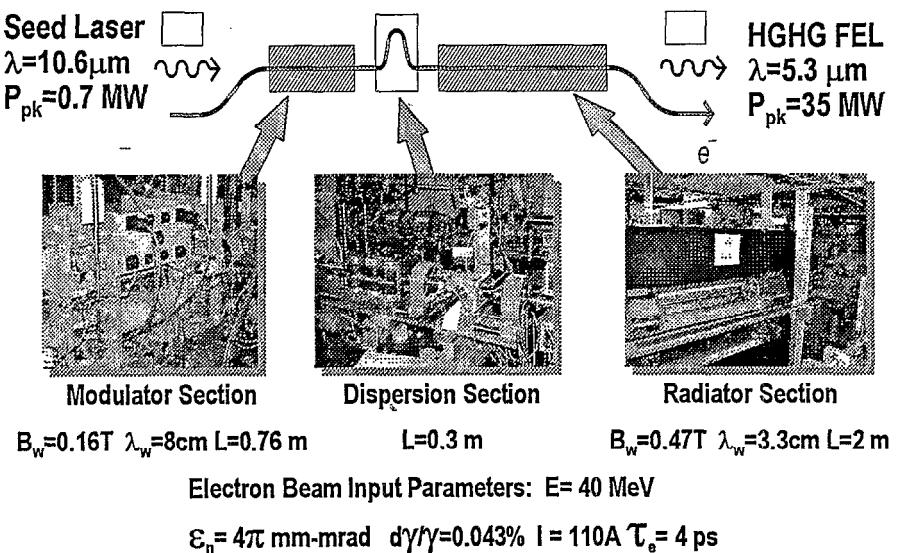


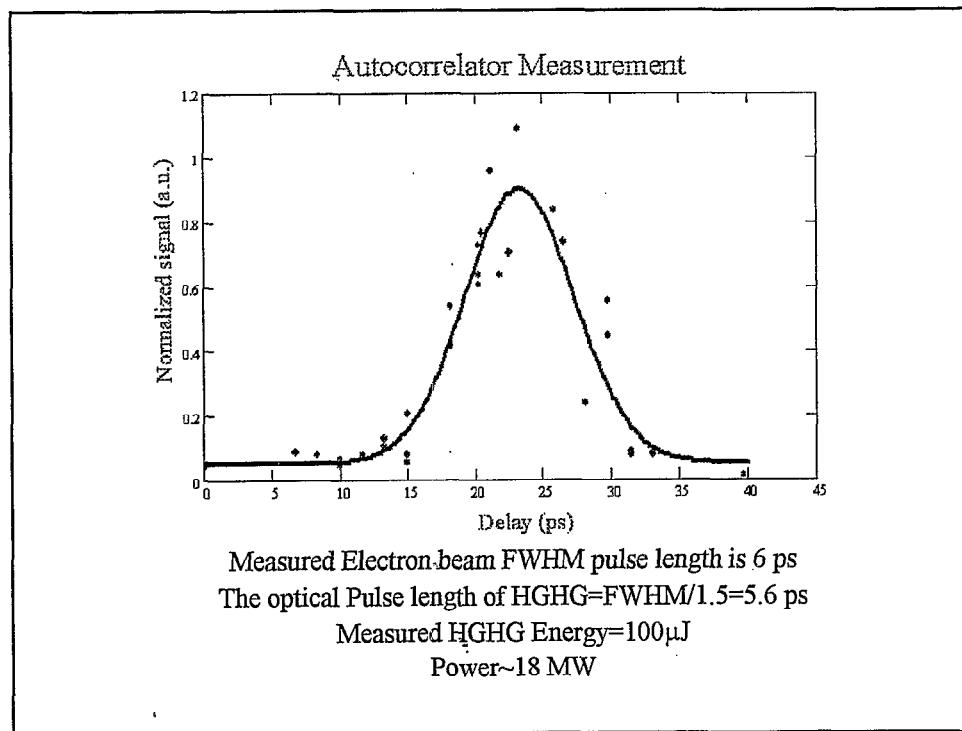
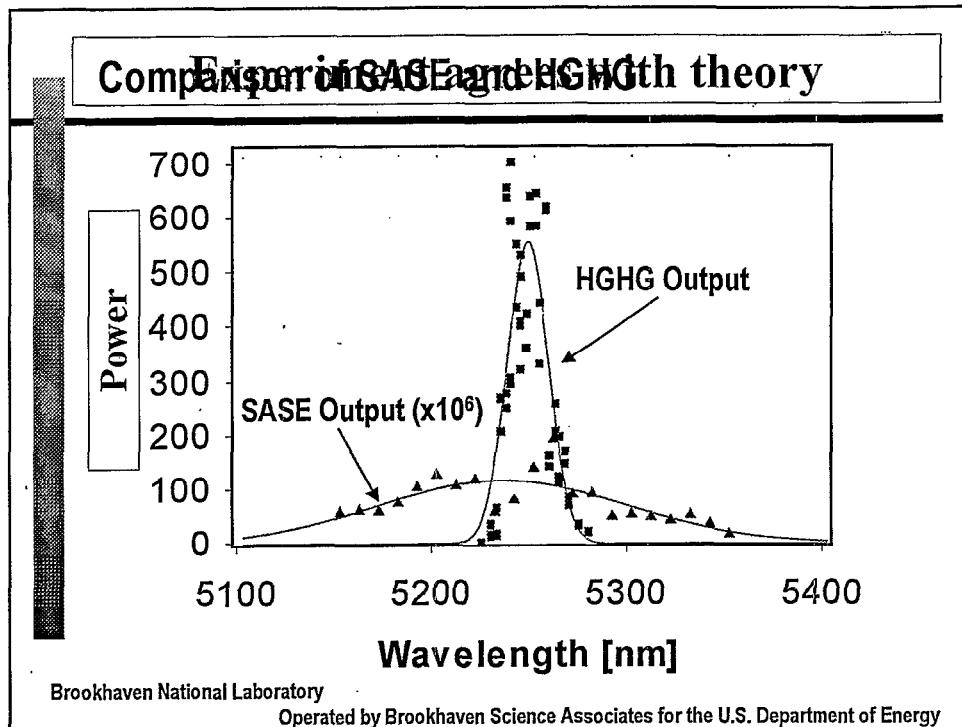
HIGH GAIN HARMONIC GENERATION



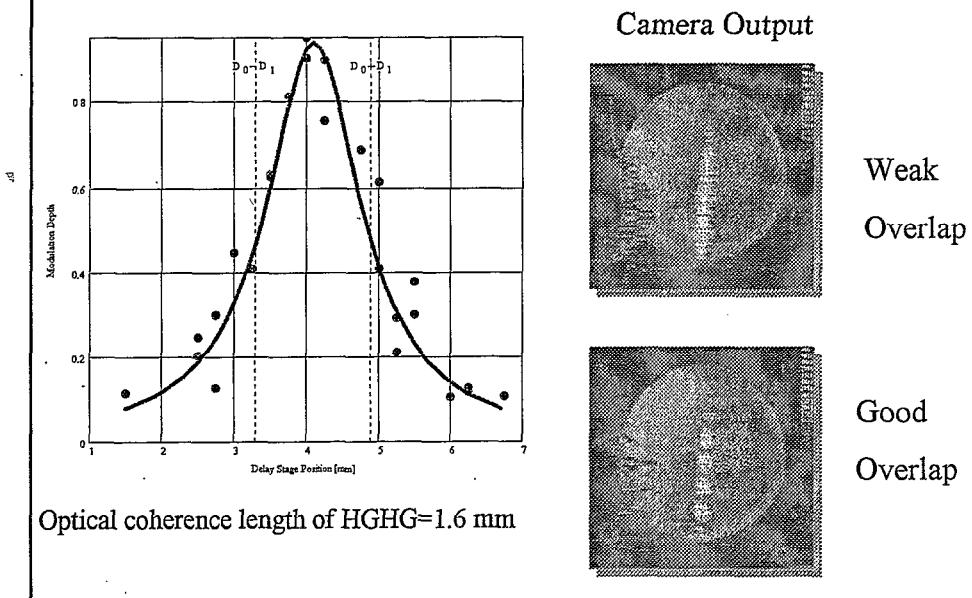
- Analogous to compression in short pulse generation
- Use harmonic to achieve shorter wavelength
- Characteristics of the input seed is impressed on e-beam
- Harmonic is amplified exponentially

The HGHG Experiment





Pulse Coherence Length Measurement using Michelson Interferometer



Advantages of HGHG

- Longitudinally fully coherent;
- Order-of-magnitude narrower bandwidth;
- Larger ratio of output/spontaneous radiation
- Central wavelength is stable;
- Pulse length is controllable;
- Output fluctuation can be reduced.

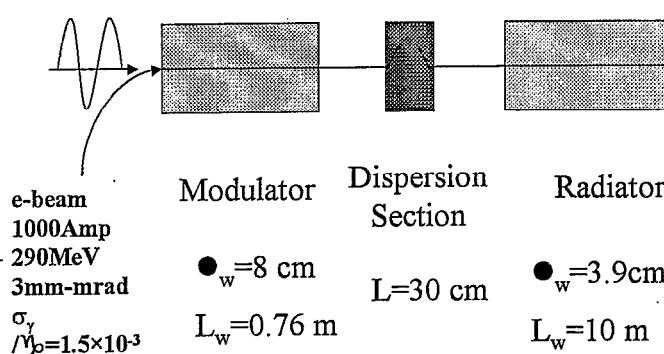
DUVFEL

$P_{in} = 90\text{MW}$

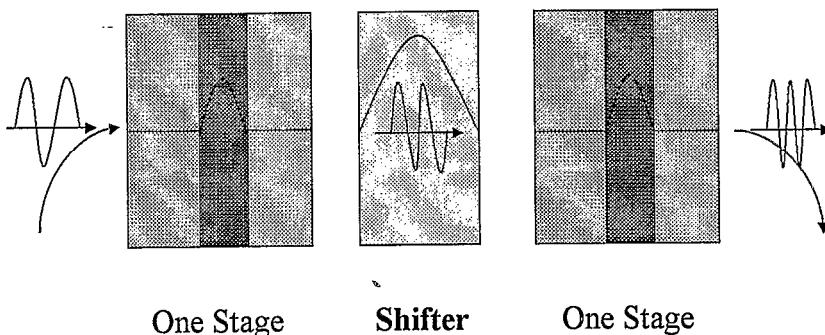
3000(Å)

$P_{out} = 130\text{MW}$

1000(Å)



Two Stages with a Shifter



Fresh Bunch Technique

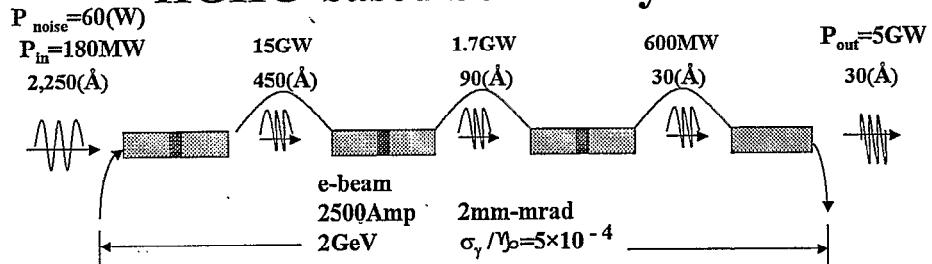
- 1. Same Bunch



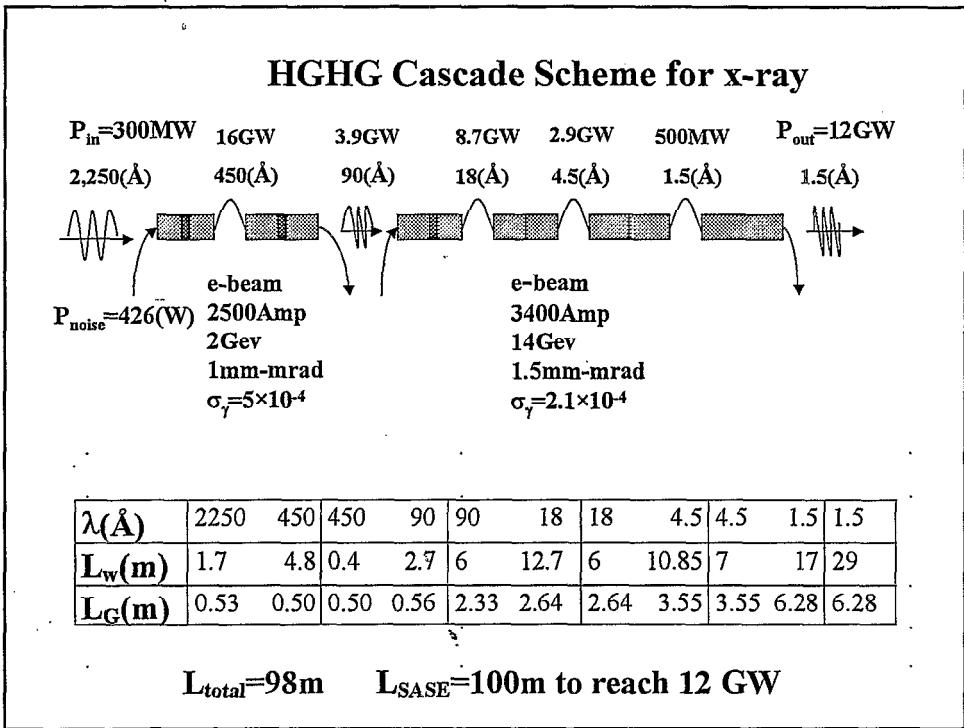
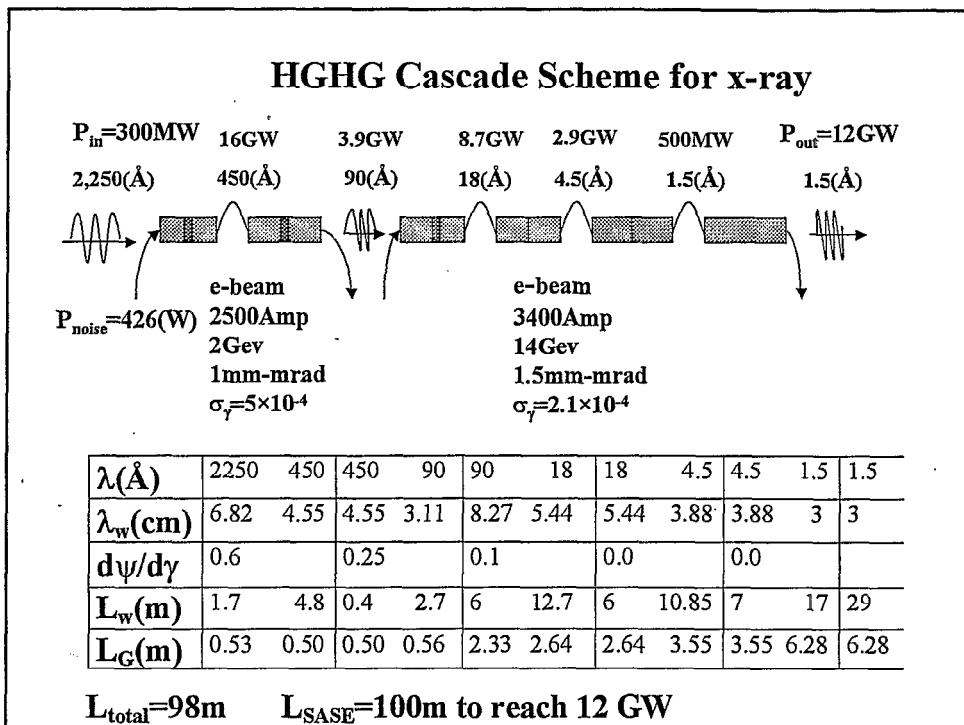
- 2. Different Bunches



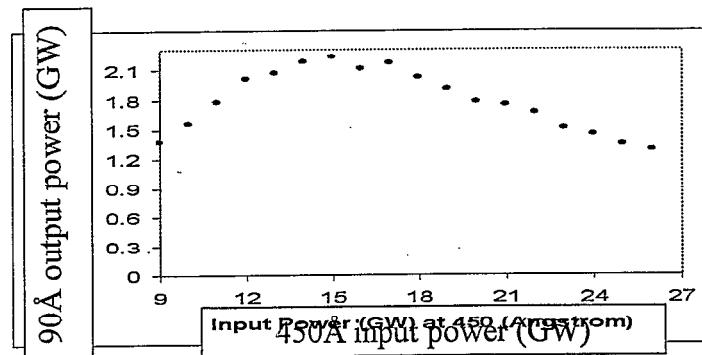
HGHG-based Soft X-ray Device



| | 1 st Stage | 2 nd Stage | 3 rd Stage | Amplifier |
|--------------------------|-----------------------|-----------------------|-----------------------|--------------------|
| $\lambda(\text{\AA})$ | 2250 | 450 | 90 | 30 |
| $\lambda_w(\text{cm})$ | 6.9 | 4.6 | 3.2 | 2.4 |
| $d\psi/dy$ | 0.49 | 0.11 | 0.04 | |
| σ_γ / γ | 5×10^{-4} | 5×10^{-4} | 5×10^{-4} | 5×10^{-4} |
| $L_w(\text{m})$ | 2.7 | 6 | 0.7 | 4 |
| $L_G(\text{m})$ | 0.6 | 0.6 | 0.6 | 0.7 |
| L_{total} | 26m | to reach 5 GW | | |

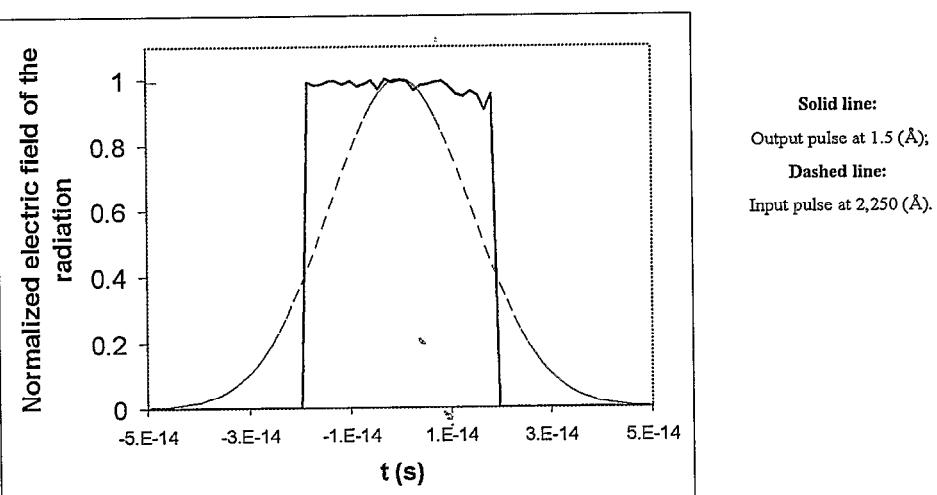


Output vs. Input Power of the 2nd Stage



- When input (450Å) varies by factor of 3, the output (90Å) only fluctuates by 30%
- Cascading scheme improves the stability

Output pulse shape, pulse length



Parameters for FELs of Several Wavelengths

| | Wavelength | Output Power | Pulse Length | Energy of e-beam | Wiggler Length | Band width |
|------------|------------|--------------|--------------|------------------|----------------|--------------------|
| DUV | 1000Å | 70MW | 1ps | 290MeV | 11 m | 3×10^{-4} |
| Soft x-ray | 30Å | 5GW | 10-40fs | 2GeV | 26 m | 3×10^{-4} |
| Hard x-ray | 1.5Å | 15GW | 10-40fs | 10-14GeV | 90-100m | 2×10^{-5} |

Conclusion

- HGHG provides a route to temporally coherent output
- We performed an experimental demonstration of the HGHG concept
- Experiment and theory show good agreement
- Cascading scheme are viable to fully coherent x-ray pulses

“Science”

Jerry Hastings

Outline

Introduction

X-Ray FEL Science

Warm Dense Matter

Structure of Biomolecules

Nanoscale Dynamics

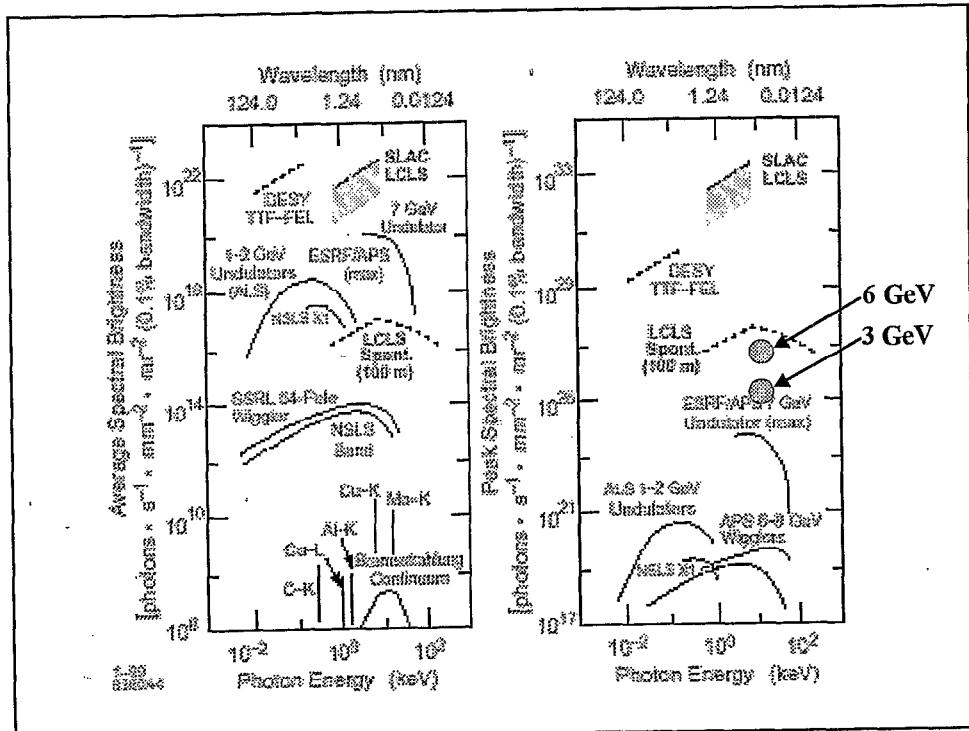
Femtochemistry

What can an energy recovery
linac source do ?

Summary

Design parameters of the LCLS

| | | |
|------------------------|----------------------|----------------------|
| Wavelength range | 15 Å | 15 Å |
| Peak sat. power | 11 GW | 9 GW |
| Coherent photons/pulse | 2.2×10^{13} | 2.2×10^{12} |
| Energy bandwidth | 0.42 % | 0.21 % |
| Pulse width | 230 fs | 230 fs |



Slides from LCLS Science case:

Warm Dense Matter

R. Lee

Structure of Biomolecules J. Hajdu

Nanoscale Dynamics

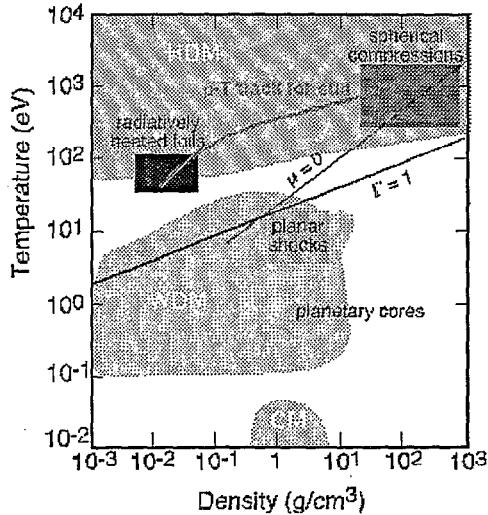
B. Stephenson

Femtochemistry

D. Imre

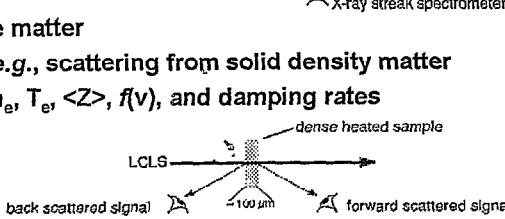
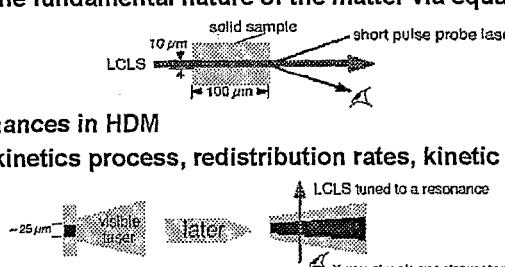
The Importance of these States of Matter Derives from their Wide Occurrence

- Hot Dense Matter (HDM) occurs in:
 - Supernova, stellar interiors, accretion disks
 - Plasma devices: laser produced plasmas, Z-pinches
 - Directly driven inertial-fusion plasma
- Warm Dense Matter (WDM) occurs in:
 - Cores of large planets
 - Systems that start solid and end as a plasma
 - X-ray driven inertial fusion implosion



Highlight of Three Experimental Areas in the High-Density Finite-temperature Regime

- Creating WDM
 - Generate ≤ 10 eV solid density matter
 - Measure the fundamental nature of the matter via equation of state
- Probing resonances in HDM
 - Measure kinetics process, redistribution rates, kinetic models
- Probing dense matter
 - Perform, e.g., scattering from solid density matter
 - Measure n_e , T_e , $\langle Z \rangle$, $f(v)$, and damping rates



Structural biology: The damage problem

BIOLOGICAL SAMPLES ARE HIGHLY RADIATION SENSITIVE

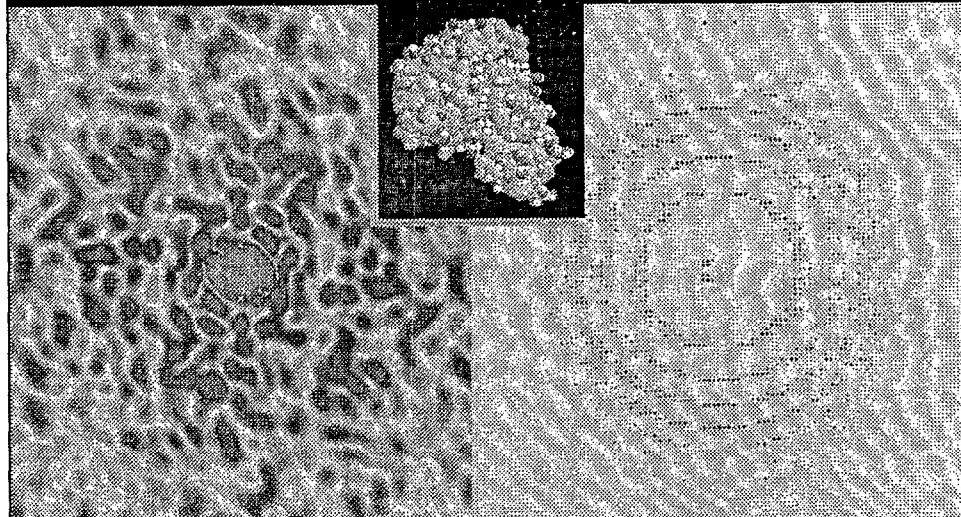
CONVENTIONAL METHODS CANNOT ACHIEVE ATOMIC
RESOLUTION on NON-REPETITIVE (or non-reproducible)
STRUCTURES

The LIMIT to DAMAGE TOLERANCE is about 200 X-ray photons/ \AA^2 in
crystals (conventional experiments)

**THE CONVENTIONAL DAMAGE BARRIER CAN BE STRETCHED by
VERY FAST IMAGING**

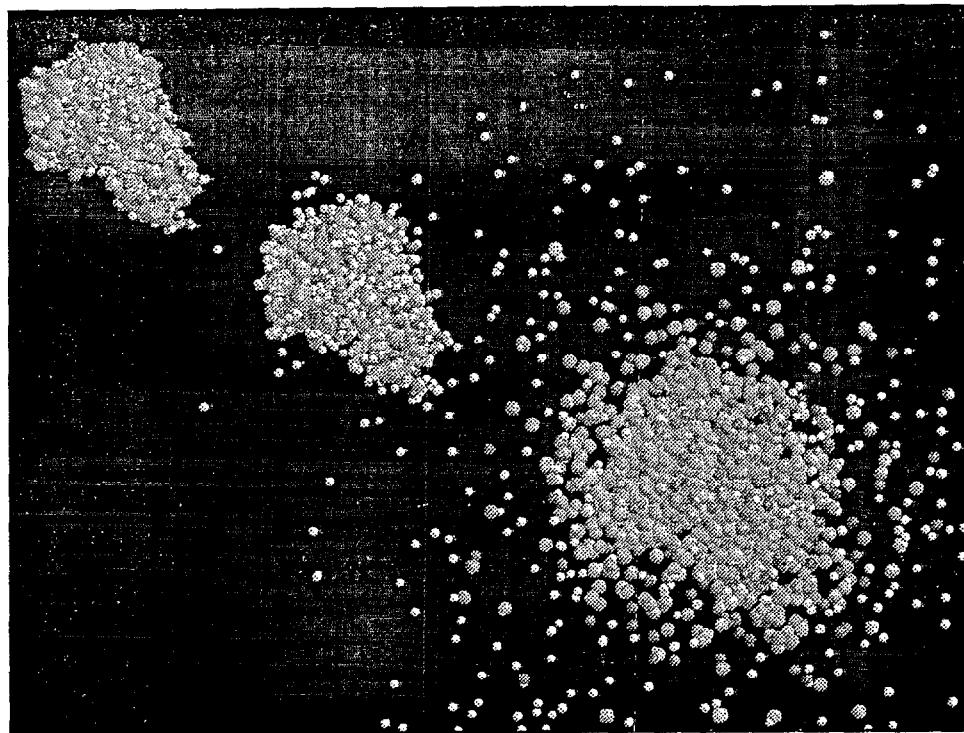
(Neutze, R., Wouts, R., van der Spoel, D., Weckert, E. Hajdu, J. (2000) *Nature* 406, 752-757)

Scattering by a single molecule and by a crystal



single molecule

crystal

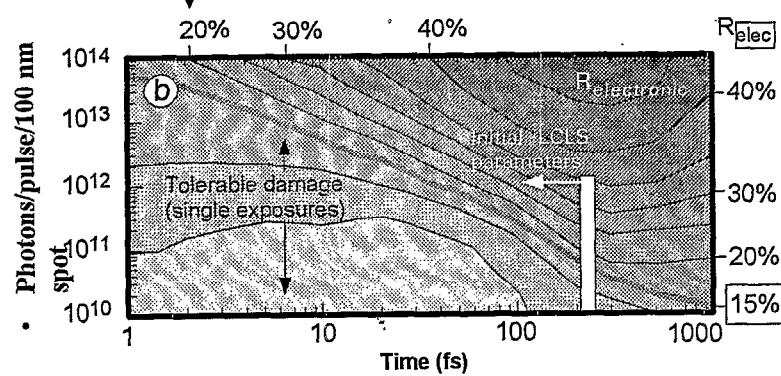


Landscape of damage tolerance

Ionisation and subsequent sample explosion cause diffraction intensities to change

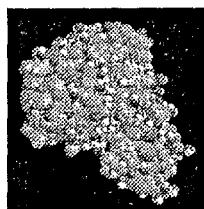
$$\text{Agreement factor} R = \frac{\sqrt{I(t)} - \sqrt{I_0}}{\sqrt{I_0}}$$

Crystallographic R-factor for proteins in the PDB

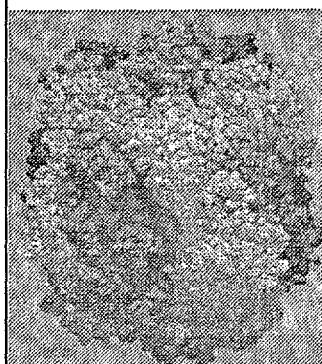


Sample size and scattering

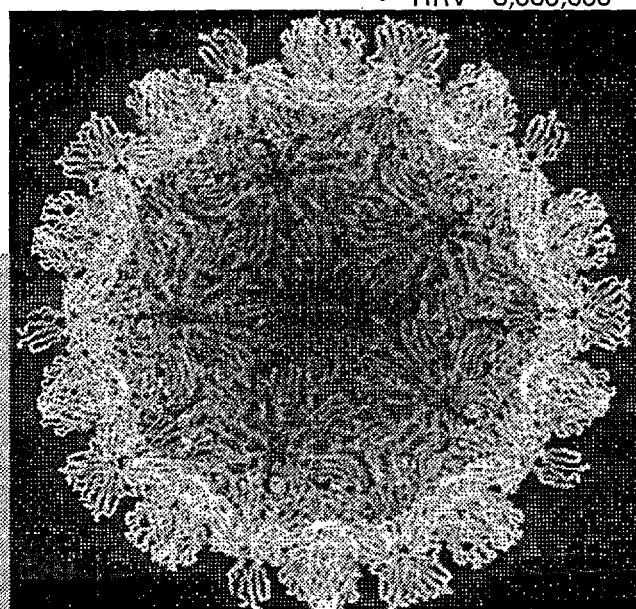
- LYSOZYME 19,806



- RUBISCO 562,000



- HRV ~3,000,000



Calculated limits of resolution with

$$R_{\text{electronic}} = 15 \%$$

| Pulse duration (FWHM) | 10 fs | 50 fs | 100 fs | 230 fs |
|---|--------------------|--------------------|--------------------|--------------------|
| Photons/pulse (100 nm spot) (R = 15%) | 5×10^{12} | 8×10^{11} | 3×10^{11} | 5×10^{10} |
| Single lysozyme molecule MW: 19,806 | 26 Å | 30 Å | >30 Å | >30 Å |
| 3x3x3 cluster of lysozymes Total MW: 535,000 | <20 Å | 3.0 Å | 6.5 Å | 12 Å |
| Single RUB ISCO molecule MW: 562,000 | 2.6 Å | 4.0 Å | 20 Å | 30 Å |
| Single viral capsid (TBSV) MW: ~3,000,000 | <20 Å | <20 Å | <20 Å | 2.4 Å |

Single virus particles look very promising

Scattering Techniques for Equilibrium Dynamics

Existing techniques

Probe thermal fluctuations:

Excite and probe fluctuations:

Title: LCLSdierkerd.eps

Creator: MATLAB, The Mathworks, Inc.

Preview: This EPS picture was not saved with a preview (TIFF or PICT).

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Scattering Techniques for Equilibrium Dynamics

XPCS and XTGS

Probe thermal fluctuations:

Excite and probe fluctuations:

Title: LCLSdierkerc.eps

Creator: MATLAB, The Mathworks, Inc.

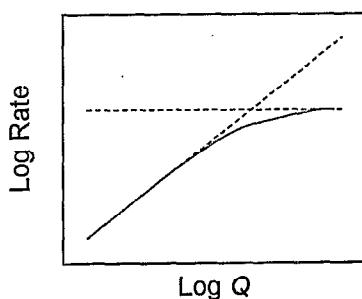
Preview: This EPS picture was not saved with a preview (TIFF or PICT).

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Advantages of Scattering Techniques

To understand dynamics, need *in-situ* techniques which resolve both *length* and *time*

Determining nature of rate-limiting step from wavenumber (Q) dependence of rate:

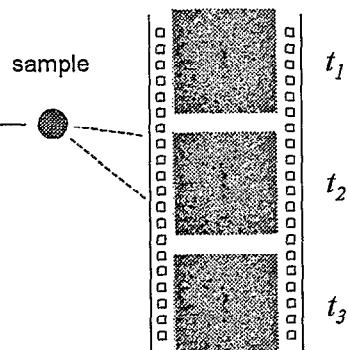
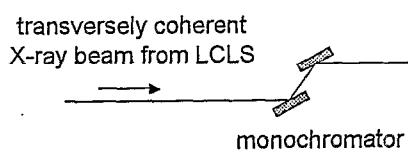


Rate $\propto Q^2$:
e.g. composition change
by diffusion
(conserved quantity)

Rate indep. of Q :
e.g. deformation
by viscous flow
(non-conserved quantity)

Experiment 1: X-ray Photon Correlation Spectroscopy (XPCS)

In milliseconds - seconds range:
Uses high *average* brilliance



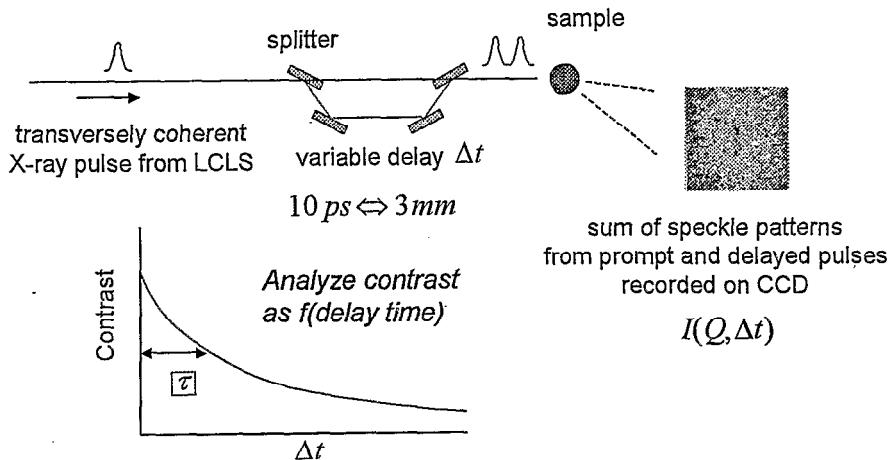
$$g_2(\Delta t) = \frac{\langle I(t)I(t + \Delta t) \rangle}{\langle I \rangle^2}$$

$$\tau^{-1}(Q) = \text{Rate}(Q)$$

"movie" of speckle
recorded by CCD
 $I(Q, t)$

Experiment 2: XPCS Using Split Pulse

In picoseconds - nanoseconds range:
Uses high peak brilliance

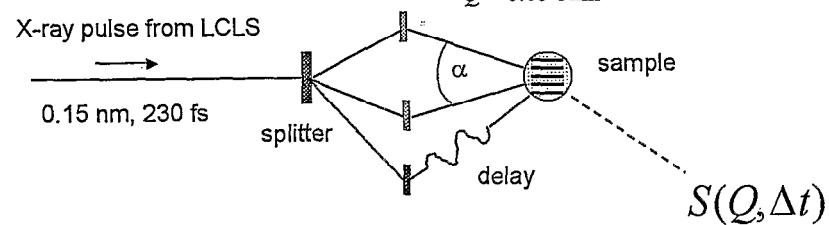


Experiment 3: X-Ray Transient Grating Spectroscopy

In picoseconds - nanoseconds range:
Uses high peak intensity

$$\alpha = 0.1-10^\circ$$

$$Q = 0.05-5 \text{ nm}^{-1}$$

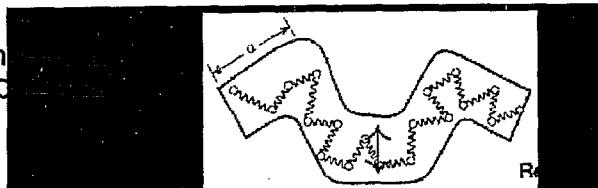


Drive system with chosen Q ,
observe response as $f(\text{delay time})$

Example: Test of Reptation Model

Dynam
Long-C

Neutron
has been
observe
motions

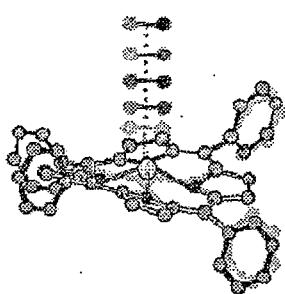


Reptation "entanglement time"

dependent of Q

CS at LCLS
would allow test of
reptation model

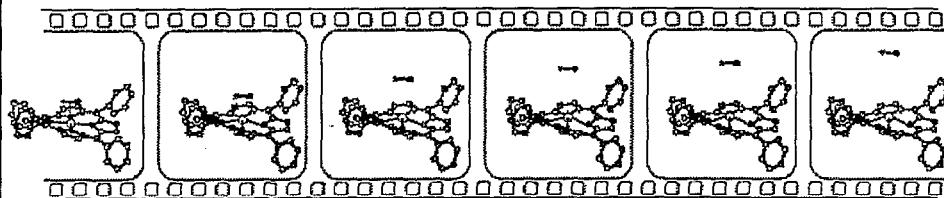
Chemistry is about Motion



Chemical transformations are about dynamics, i.e. rapid changes in bond lengths and bond angles.

What is needed is a tool that will make possible a simple connection between the static picture and its time evolution.

Chemistry is about Motion



The ultimate goal of any molecular dynamics study is to produce a motion picture of the nuclear motions as a function of time.

Spectroscopy of the Transition State

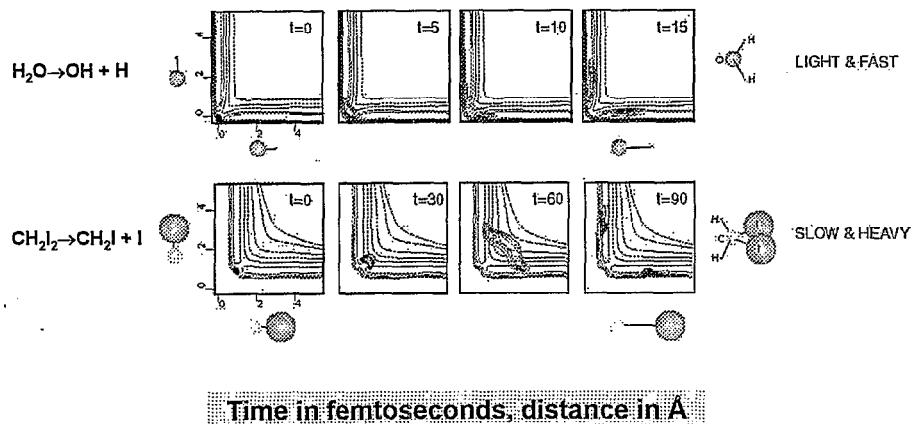
Capturing molecules *in the process of reacting* has been a long-time dream

Femtosecond lasers are fast enough

BUT

Their greater than 200-nm wavelength does not allow for any spatial information

Temporal and Spatial Scales



UED Experimental Set-up

Ultrafast Electron Diffraction
H. Zewail

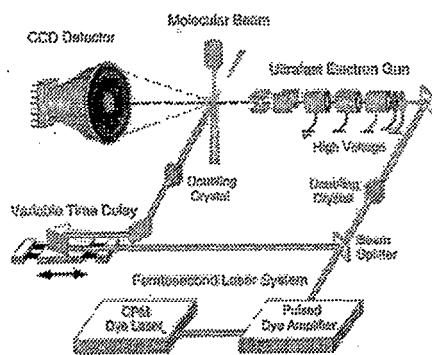
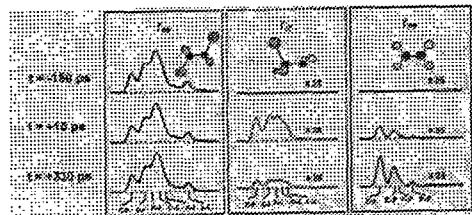
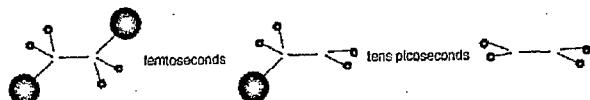


Fig. 1. A schematic of the experimental setup used for ultrafast electron diffraction (UED).

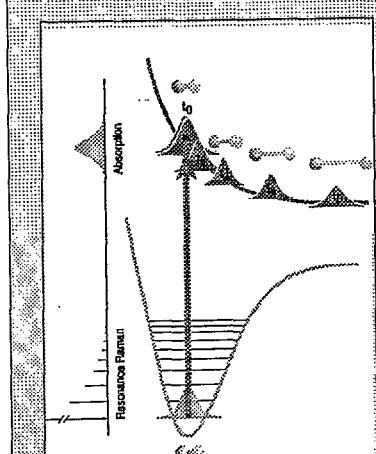
UED $\text{CH}_2\text{I}-\text{CH}_2\text{I}$ Photodissociation



UED will never break the psec time limit because of the fundamental relationship between the number of electrons in the bunch and pulse length.

The LCLS is the only tool with the required temporal and spatial resolution

Gas phase photodissociation reactions



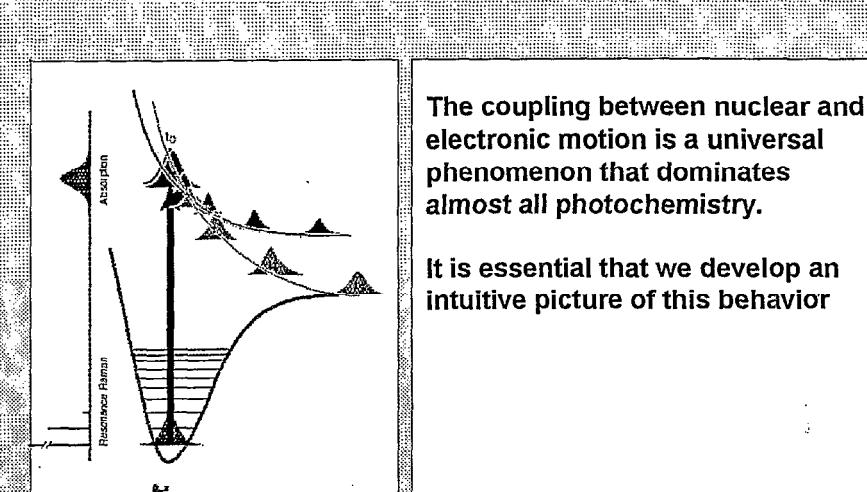
Photodissociation of an isolated diatomic molecule is the simplest of chemical reactions.

$t=0$ is easily defined

The initial wave-function is well defined

The wave-function remains localized throughout the reaction

Nuclear and Electronic Coupling is Universal Phenomenon



Comparison between UED and LCLS

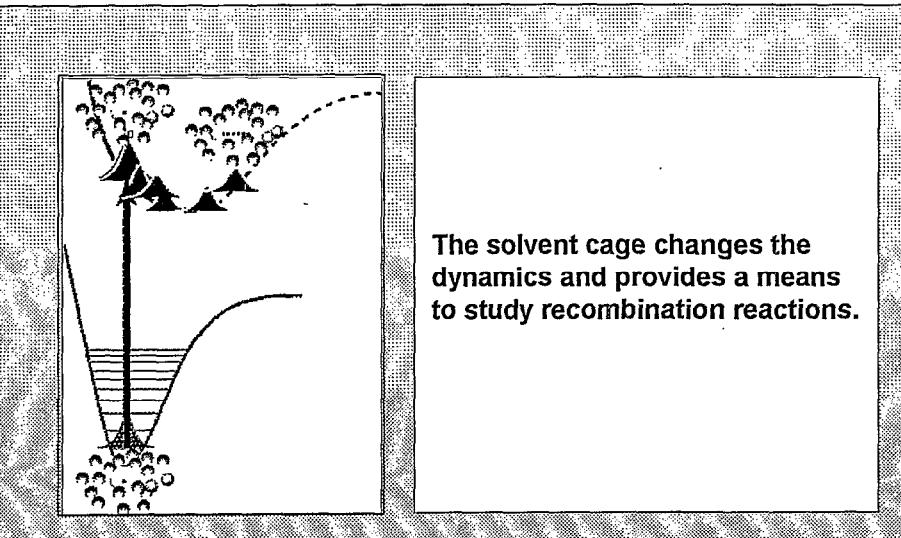
Comparison between Ultrafast Electron Diffraction (UED) and the LCLS

| | Δt^1 | Flux | Cross section ² | Rate Hz | Signal ³ |
|------|--------------|-------------------|----------------------------|---------|---------------------|
| UED | 10ps | 7000 | 10^7 | 1000 | $7 \cdot 10^{13}$ |
| LCLS | 200fs | $2 \cdot 10^{12}$ | 1 | 100 | $2 \cdot 10^{14}$ |

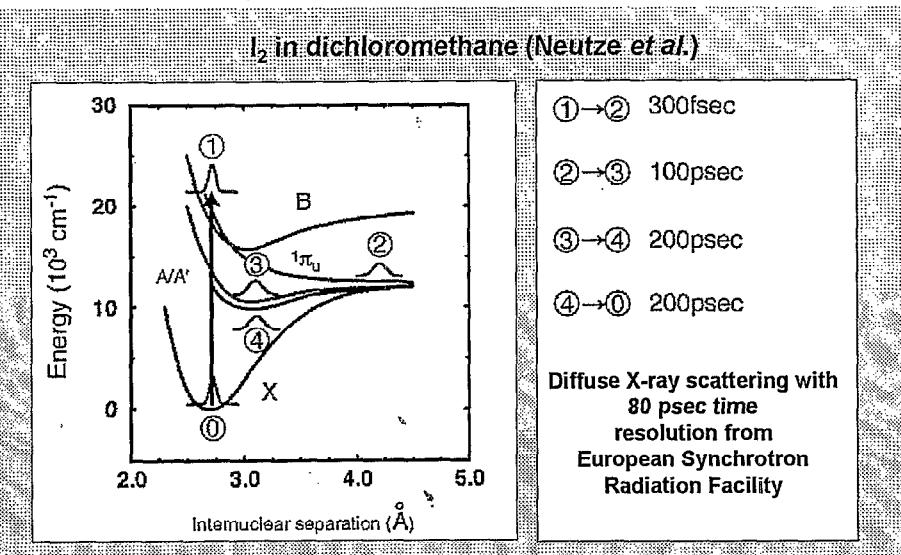
¹ time resolution; ² relative crosssection; ³ relative signals

The predicted signals are comparable but the LCLS time resolution is at least 50 times better.

Experiment 2. Condensed phase photochemistry

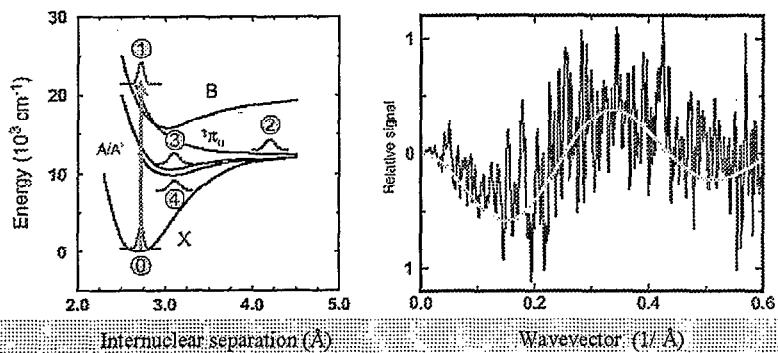


Third Generation Sources Have a Limited Time Resolution

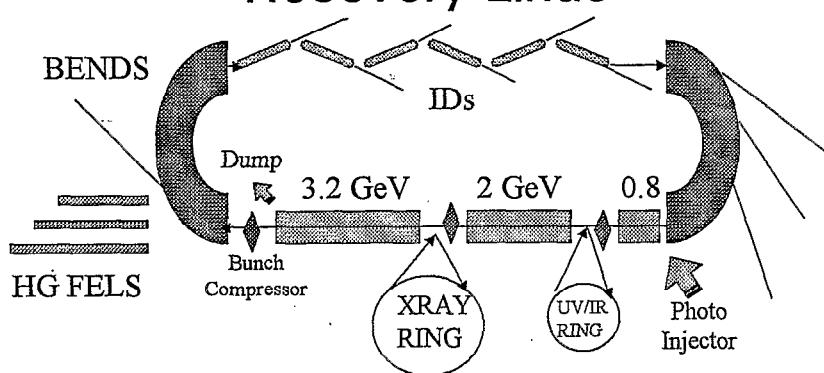


An Example from ESRF

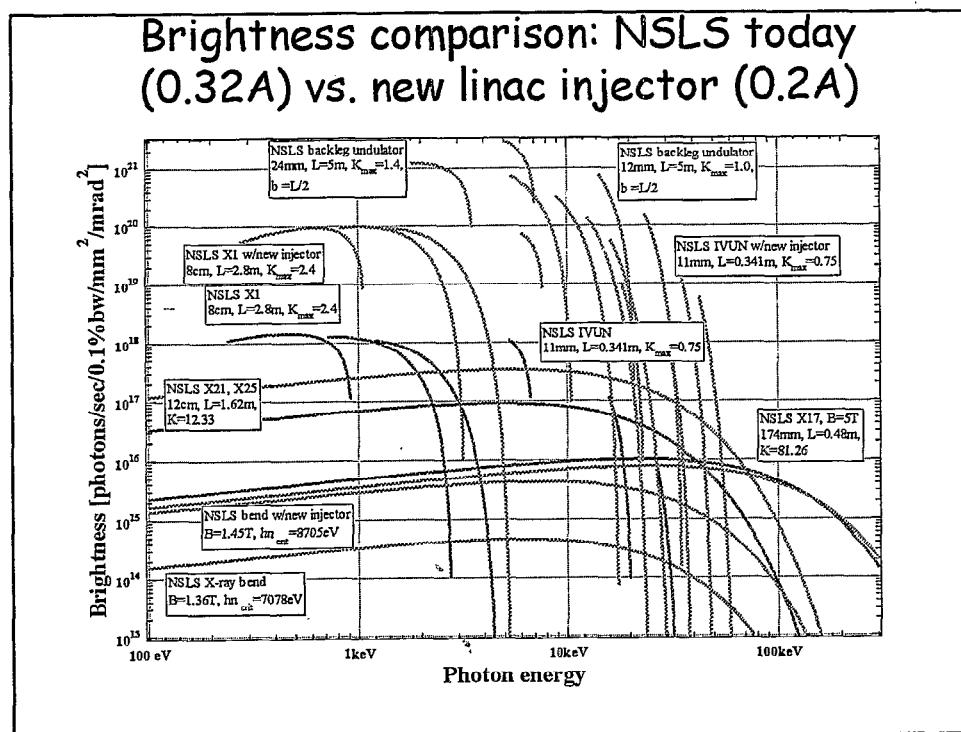
I₂ in dichloromethane (Neutze et al.)



6 GeV Single Pass Energy Recovery Linac

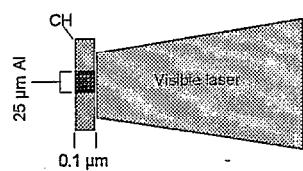


| | Pulse length | Photons/pulse |
|-----------------|--------------|--------------------|
| ALS pulse slice | 300 fs | 10 |
| 3 GeV ERL | 10 fs | few $\times 10^6$ |
| 6 GeV ERL | 10 fs | few $\times 10^7$ |
| LCLS | 230 fs | 2×10^{12} |



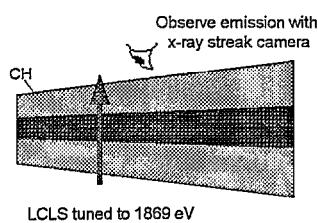
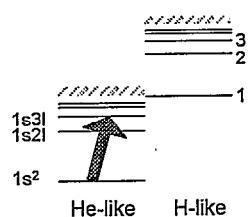
LCLS Will Create Excitation Levels That Are Observable in Emission

• Schematic experiment

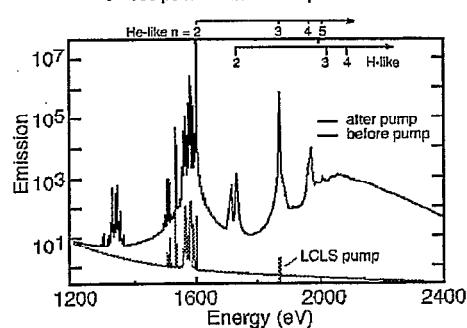


• t = 0 laser irradiates Al dot

• Simulations

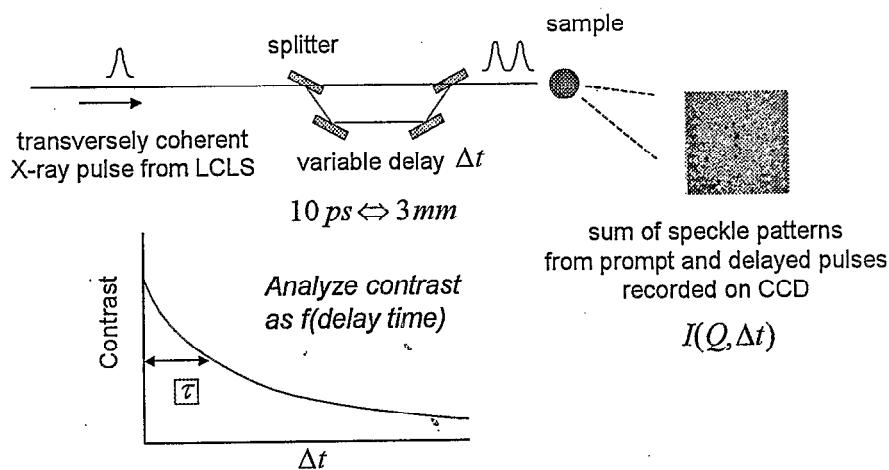


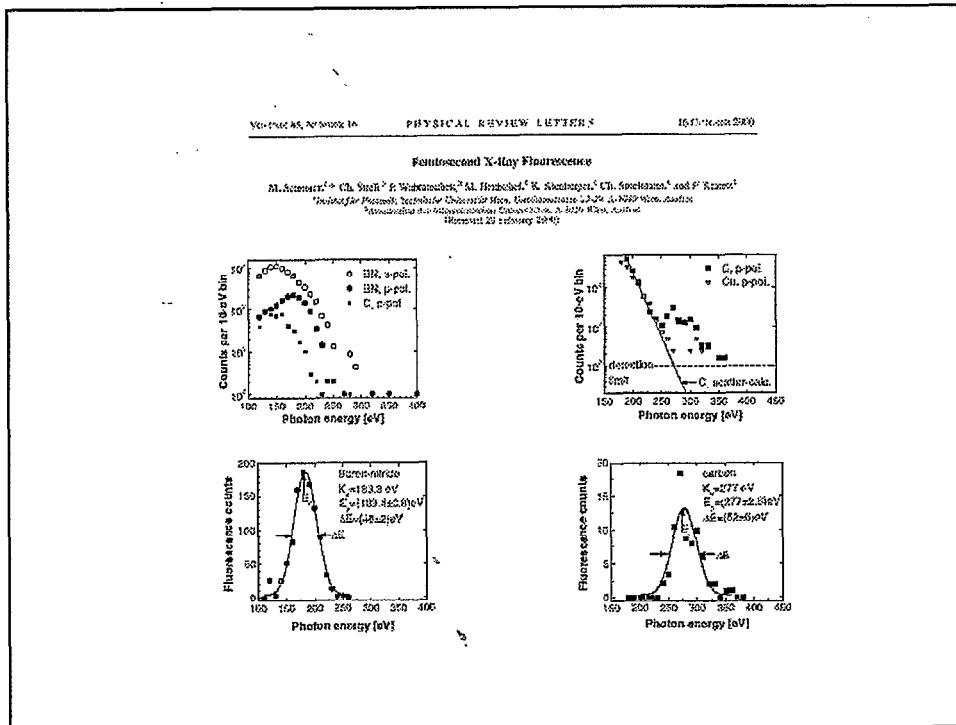
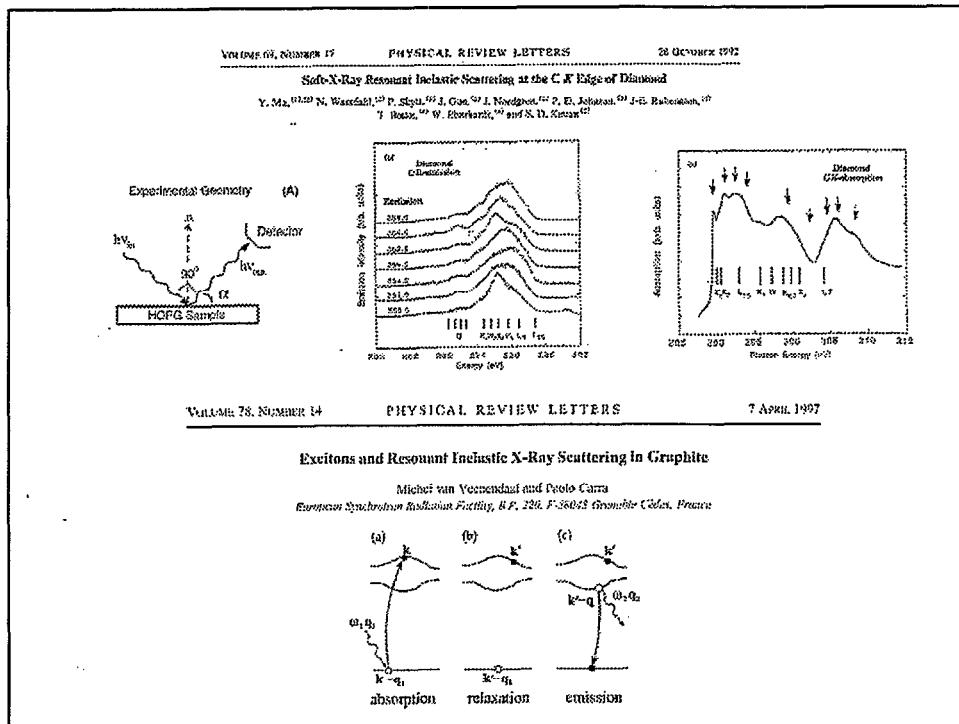
• t = 100 ps LCLS irradiates plasma



Experiment 2: XPCS Using Split Pulse

In picoseconds - nanoseconds range:
Uses high peak brilliance





| | Energy Recover Linac | LCLS XFEL | HGHG XFEL |
|-----------------------|----------------------------|--------------|--------------|
| Warm Dense Matter | probe only | yes | yes |
| Biomolecules | no | start | yes |
| Nanoscale Dynamics | start | yes | yes |
| Femtochemistry | start | start | yes |

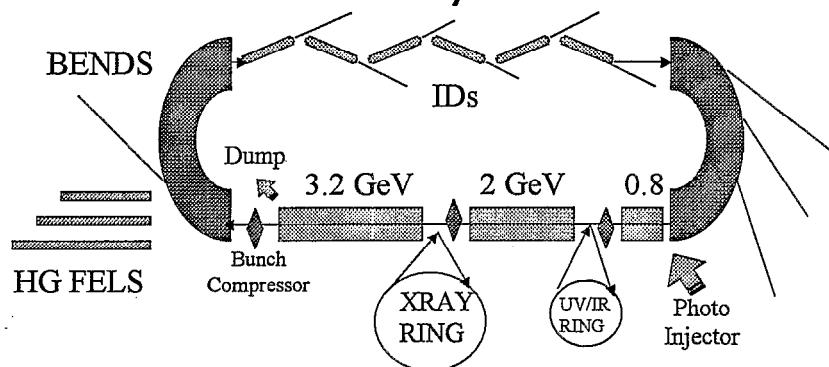
Summary

Maintain the NSLS as an intellectual center.

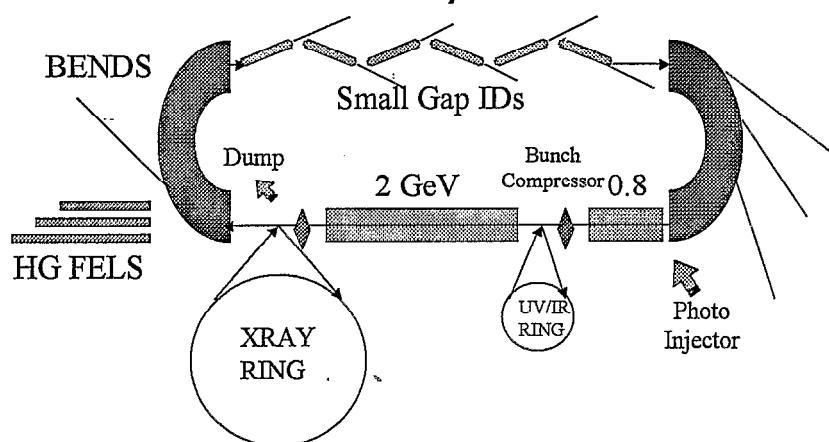
Start science based access.

Develop a detailed plan for a new source based on an energy recovery linac.

6 GeV Single Pass Energy Recovery Linac



2.8 GeV Single Pass Energy Recovery Linac



7 GeV Multi-Pass Energy Recovery Linac

